



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:41 AM UTC

PDB ID : 1P7Y / pdb_00001p7y
Title : Crystal structure of the D181A variant of catalase HP11 from E. coli
Authors : Chelikani, P.; Carpena, X.; Fita, I.; Loewen, P.C.
Deposited on : 2003-05-06
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

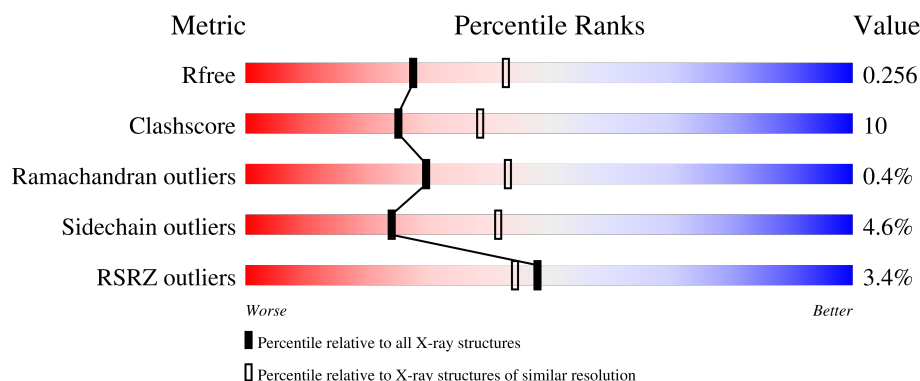
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	753	5% 67% 24% ...
1	B	753	% 62% 28% 6% ..
1	C	753	% 65% 26% 5% .
1	D	753	6% 63% 28% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25927 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	1	0
			5747	3648	1006	1081	12			
1	B	727	Total	C	N	O	S	0	1	0
			5747	3648	1006	1081	12			
1	C	727	Total	C	N	O	S	0	1	0
			5747	3648	1006	1081	12			
1	D	727	Total	C	N	O	S	0	1	0
			5747	3648	1006	1081	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	ALA	ASP	engineered mutation	UNP P21179
B	181	ALA	ASP	engineered mutation	UNP P21179
C	181	ALA	ASP	engineered mutation	UNP P21179
D	181	ALA	ASP	engineered mutation	UNP P21179

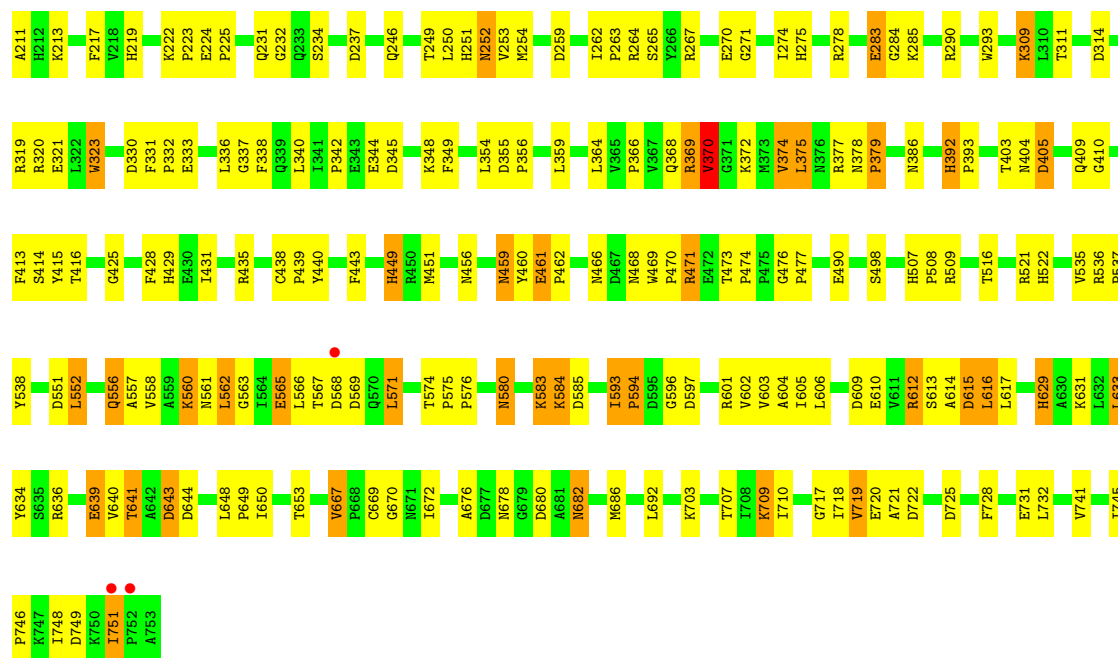
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



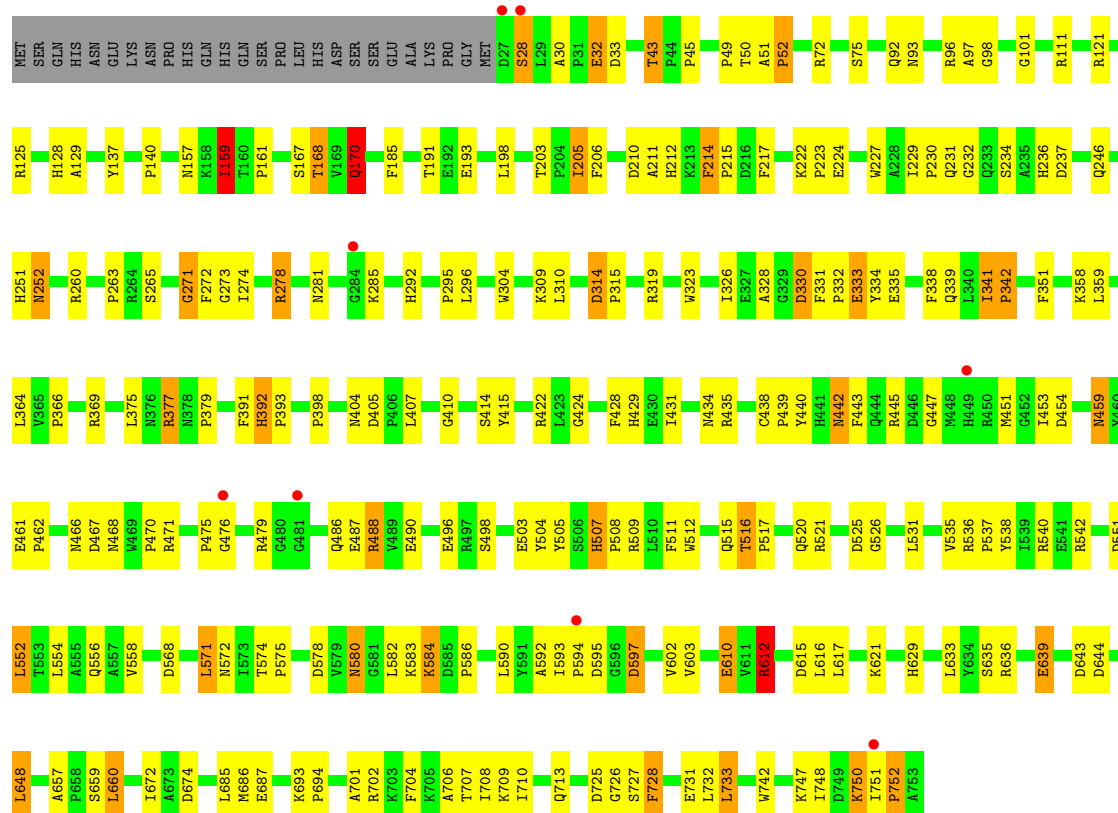
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	732	Total O 732 732	0	0
3	B	641	Total O 641 641	0	0
3	C	673	Total O 673 673	0	0
3	D	721	Total O 721 721	0	0

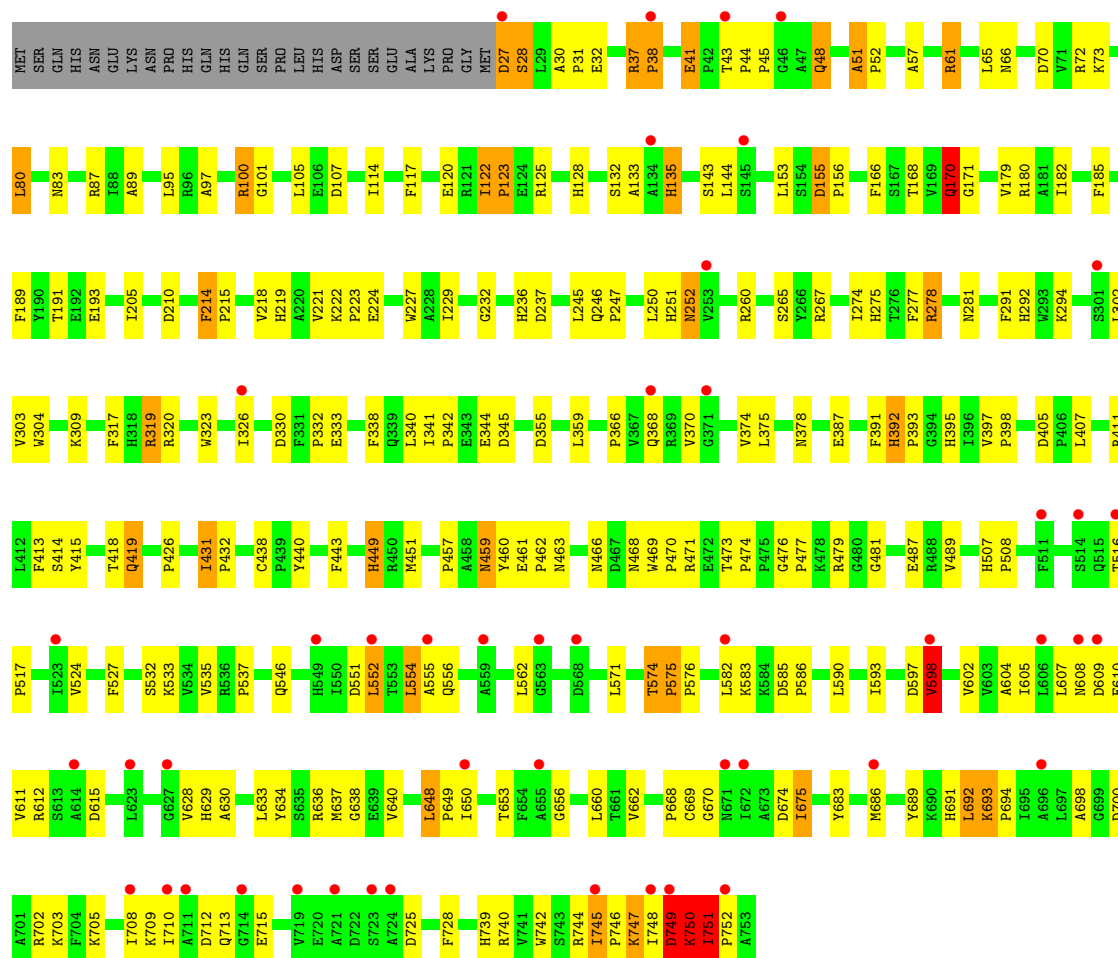


• Molecule 1: Catalase HP11



• Molecule 1: Catalase HP11





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.29Å 132.86Å 121.75Å 90.00° 109.40° 90.00°	Depositor
Resolution (Å)	29.80 – 2.40 29.80 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.80-2.40) 96.6 (29.80-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.144 , 0.225 0.209 , 0.256	Depositor DCC
R_{free} test set	5332 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 75.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	25927	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.72	0/5908	1.82	141/8032 (1.8%)
1	B	0.71	0/5908	1.84	156/8032 (1.9%)
1	C	0.71	0/5908	1.88	144/8032 (1.8%)
1	D	0.71	0/5908	1.85	155/8032 (1.9%)
All	All	0.71	0/23632	1.85	596/32128 (1.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (596) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	612	ARG	CD-NE-CZ	34.71	173.00	124.40
1	D	479	ARG	CD-NE-CZ	17.86	149.41	124.40
1	D	612	ARG	CD-NE-CZ	15.07	145.50	124.40
1	C	595	ASP	CA-CB-CG	14.99	127.59	112.60
1	D	474	PRO	N-CA-CB	12.94	109.95	103.22
1	C	728	PHE	CA-CB-CG	12.77	126.57	113.80
1	D	575	PRO	N-CA-CB	12.38	110.12	103.19
1	C	414	SER	N-CA-C	11.74	123.64	111.07
1	D	449	HIS	CA-CB-CG	11.21	125.01	113.80
1	A	414	SER	N-CA-C	10.86	123.20	111.36
1	C	726	GLY	N-CA-C	-10.81	92.58	110.95
1	D	27	ASP	CA-CB-CG	10.64	123.24	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170[A]	GLN	CA-CB-CG	10.56	135.22	114.10
1	C	170[B]	GLN	CA-CB-CG	10.56	135.22	114.10
1	B	27	ASP	CA-C-N	10.43	141.47	121.54
1	B	27	ASP	C-N-CA	10.43	141.47	121.54
1	B	601	ARG	CD-NE-CZ	10.42	138.99	124.40
1	D	725	ASP	CA-CB-CG	10.38	122.97	112.60
1	B	37	ARG	CD-NE-CZ	10.25	138.75	124.40
1	B	37	ARG	NE-CZ-NH2	10.21	128.38	119.20
1	D	749	ASP	CA-CB-CG	9.90	122.50	112.60
1	C	597	ASP	CA-CB-CG	9.79	122.39	112.60
1	A	497	ARG	NE-CZ-NH1	9.77	131.27	121.50
1	C	210	ASP	CA-CB-CG	9.40	122.00	112.60
1	A	728	PHE	CA-CB-CG	9.24	123.04	113.80
1	A	43	THR	CA-C-N	9.12	126.32	119.66
1	A	43	THR	C-N-CA	9.12	126.32	119.66
1	D	61	ARG	CD-NE-CZ	9.04	137.06	124.40
1	A	474	PRO	N-CA-CB	8.99	108.23	103.19
1	D	170[A]	GLN	CA-CB-CG	8.96	132.02	114.10
1	D	170[B]	GLN	CA-CB-CG	8.96	132.02	114.10
1	B	414	SER	N-CA-C	8.83	120.52	111.07
1	C	575	PRO	N-CA-CB	8.78	107.78	103.22
1	D	391	PHE	CA-CB-CG	8.75	122.55	113.80
1	A	338	PHE	CA-CB-CG	8.66	122.46	113.80
1	C	725	ASP	N-CA-CB	8.65	125.11	110.49
1	D	414	SER	N-CA-C	8.63	120.69	111.28
1	C	121	ARG	CD-NE-CZ	8.58	136.41	124.40
1	C	428	PHE	CA-CB-CG	-8.57	105.23	113.80
1	C	725	ASP	CA-CB-CG	-8.54	104.06	112.60
1	A	44	PRO	N-CA-CB	8.53	107.97	103.19
1	D	338	PHE	CA-CB-CG	8.51	122.31	113.80
1	C	28	SER	N-CA-C	-8.47	99.19	111.30
1	D	189	PHE	CA-CB-CG	8.47	122.27	113.80
1	A	341	ILE	CA-C-O	8.39	124.30	119.94
1	B	270	GLU	CA-C-N	8.36	128.04	121.61
1	B	270	GLU	C-N-CA	8.36	128.04	121.61
1	D	597	ASP	CA-CB-CG	8.35	120.95	112.60
1	D	574	THR	CA-C-N	8.32	125.73	119.66
1	D	574	THR	C-N-CA	8.32	125.73	119.66
1	B	580	ASN	CA-CB-CG	-8.27	104.33	112.60
1	D	185	PHE	CA-CB-CG	8.24	122.04	113.80
1	B	369	ARG	CD-NE-CZ	8.22	135.91	124.40
1	B	27	ASP	CA-CB-CG	8.19	120.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	THR	CA-C-O	-8.15	111.85	120.58
1	A	350	ASP	CB-CA-C	7.97	124.09	110.94
1	D	44	PRO	N-CA-CB	7.96	107.36	103.22
1	A	716	GLU	CB-CG-CD	7.96	126.13	112.60
1	C	471	ARG	CD-NE-CZ	-7.91	113.32	124.40
1	A	59	ASP	CA-CB-CG	7.88	120.47	112.60
1	B	314	ASP	CA-C-N	7.82	127.54	119.56
1	B	314	ASP	C-N-CA	7.82	127.54	119.56
1	C	273	GLY	CA-C-N	7.81	136.03	121.97
1	C	273	GLY	C-N-CA	7.81	136.03	121.97
1	D	546	GLN	OE1-CD-NE2	-7.80	114.80	122.60
1	A	595	ASP	CA-CB-CG	7.76	120.36	112.60
1	D	691	HIS	CA-C-O	7.71	130.12	119.80
1	B	278	ARG	CD-NE-CZ	7.70	135.17	124.40
1	B	639	GLU	CB-CG-CD	7.67	125.63	112.60
1	D	43	THR	CA-C-N	7.62	125.15	119.66
1	D	43	THR	C-N-CA	7.62	125.15	119.66
1	B	224	GLU	CA-C-N	7.60	127.24	119.19
1	B	224	GLU	C-N-CA	7.60	127.24	119.19
1	C	295	PRO	N-CA-CB	7.57	108.30	103.23
1	B	597	ASP	CA-CB-CG	7.56	120.16	112.60
1	B	575	PRO	N-CA-CB	7.52	110.37	103.08
1	D	576	PRO	N-CA-CB	7.50	107.12	103.22
1	C	422	ARG	CD-NE-CZ	7.50	134.91	124.40
1	D	527	PHE	CA-CB-CG	7.47	121.28	113.80
1	C	391	PHE	CA-CB-CG	7.46	121.26	113.80
1	B	185	PHE	CA-CB-CG	7.44	121.24	113.80
1	D	615	ASP	CA-CB-CG	7.43	120.03	112.60
1	C	674	ASP	CA-CB-CG	7.39	119.99	112.60
1	A	170[A]	GLN	CA-CB-CG	7.35	128.79	114.10
1	A	170[B]	GLN	CA-CB-CG	7.35	128.79	114.10
1	A	349	PHE	CA-CB-CG	-7.34	106.46	113.80
1	B	290	ARG	N-CA-CB	7.31	123.44	110.80
1	C	224	GLU	CA-C-O	7.31	127.77	120.17
1	D	48	GLN	O-C-N	7.25	126.35	121.71
1	A	708	ILE	CA-C-N	7.22	135.34	121.54
1	A	708	ILE	C-N-CA	7.22	135.34	121.54
1	C	272	PHE	CA-C-O	-7.18	112.73	121.06
1	A	383	PHE	CA-CB-CG	-7.17	106.63	113.80
1	B	283	GLU	CA-CB-CG	7.17	128.44	114.10
1	B	722	ASP	CA-CB-CG	-7.16	105.44	112.60
1	D	317	PHE	CA-C-O	-7.16	113.24	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ARG	NE-CZ-NH2	7.14	125.63	119.20
1	D	237	ASP	N-CA-C	7.14	119.68	111.11
1	A	713	GLN	N-CA-C	-7.14	104.57	113.28
1	A	749	ASP	CA-CB-CG	-7.14	105.46	112.60
1	A	591	TYR	N-CA-C	7.13	124.31	113.61
1	C	45	PRO	CA-C-O	7.12	129.08	121.32
1	C	496	GLU	CA-C-O	7.11	128.95	120.99
1	A	405	ASP	CA-C-N	7.10	126.73	119.56
1	A	405	ASP	C-N-CA	7.10	126.73	119.56
1	C	615	ASP	CA-CB-CG	7.10	119.70	112.60
1	B	474	PRO	N-CA-CB	7.10	107.16	103.19
1	C	338	PHE	CA-CB-CG	7.10	120.90	113.80
1	C	281	ASN	CA-CB-CG	7.03	119.63	112.60
1	A	226	HIS	CA-C-O	-6.99	113.07	120.55
1	B	170[A]	GLN	CA-CB-CG	6.99	128.07	114.10
1	B	170[B]	GLN	CA-CB-CG	6.99	128.07	114.10
1	C	217	PHE	CA-CB-CG	-6.98	106.82	113.80
1	A	422	ARG	NE-CZ-NH2	6.96	125.46	119.20
1	A	608	ASN	CA-C-O	-6.94	113.44	121.49
1	B	474	PRO	O-C-N	6.91	124.49	121.31
1	A	110	LEU	CA-C-O	-6.91	113.56	120.82
1	C	504	TYR	CA-C-O	6.90	126.62	118.69
1	A	507	HIS	O-C-N	-6.90	114.34	120.48
1	A	185	PHE	CA-CB-CG	6.89	120.69	113.80
1	D	355	ASP	CA-C-N	6.88	127.03	119.87
1	D	355	ASP	C-N-CA	6.88	127.03	119.87
1	C	377	ARG	NE-CZ-NH1	-6.88	114.62	121.50
1	A	575	PRO	N-CA-CB	6.87	106.79	103.22
1	D	691	HIS	O-C-N	-6.86	112.87	122.06
1	C	28	SER	N-CA-CB	6.85	121.57	111.43
1	D	61	ARG	NE-CZ-NH2	6.83	125.35	119.20
1	A	415	TYR	CA-C-N	6.83	129.31	120.44
1	A	415	TYR	C-N-CA	6.83	129.31	120.44
1	C	185	PHE	CA-CB-CG	6.81	120.61	113.80
1	C	475	PRO	N-CA-CB	6.79	109.35	103.31
1	B	98	GLY	N-CA-C	-6.78	104.27	112.48
1	D	387	GLU	CA-C-O	-6.78	113.64	120.90
1	D	345	ASP	CA-CB-CG	6.76	119.36	112.60
1	B	616	LEU	N-CA-CB	6.73	119.77	110.01
1	A	497	ARG	NE-CZ-NH2	-6.72	113.15	119.20
1	B	319	ARG	NE-CZ-NH2	6.72	125.25	119.20
1	A	80	LEU	CA-C-O	-6.71	113.27	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	501	PHE	CA-CB-CG	6.71	120.51	113.80
1	C	214	PHE	CA-C-N	6.70	126.29	119.19
1	C	214	PHE	C-N-CA	6.70	126.29	119.19
1	B	217	PHE	CA-CB-CG	-6.69	107.11	113.80
1	B	262	ILE	CA-C-N	6.69	126.67	119.78
1	B	262	ILE	C-N-CA	6.69	126.67	119.78
1	A	386	ASN	CA-CB-CG	6.67	119.27	112.60
1	A	314	ASP	CA-C-N	6.67	126.29	119.56
1	A	314	ASP	C-N-CA	6.67	126.29	119.56
1	D	597	ASP	CA-C-N	6.67	131.57	120.64
1	D	597	ASP	C-N-CA	6.67	131.57	120.64
1	A	541	GLU	CA-CB-CG	-6.66	100.79	114.10
1	D	236	HIS	CA-CB-CG	6.63	120.43	113.80
1	A	266	TYR	CA-C-N	6.63	130.39	120.31
1	A	266	TYR	C-N-CA	6.63	130.39	120.31
1	D	122	ILE	N-CA-CB	6.62	117.30	111.67
1	B	319	ARG	NE-CZ-NH1	-6.62	114.88	121.50
1	B	28	SER	N-CA-CB	6.60	121.65	110.49
1	A	751	ILE	N-CA-CB	6.60	117.50	110.17
1	A	349	PHE	CA-C-N	-6.60	112.11	122.73
1	A	349	PHE	C-N-CA	-6.60	112.11	122.73
1	C	52	PRO	N-CA-CB	6.59	109.12	103.19
1	D	155	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	155	ASP	CA-C-N	6.57	126.26	119.56
1	A	155	ASP	C-N-CA	6.57	126.26	119.56
1	D	728	PHE	CA-C-O	-6.56	113.88	120.90
1	A	348	LYS	N-CA-C	6.54	121.26	113.28
1	B	178	THR	N-CA-C	6.54	119.91	112.97
1	C	516	THR	CA-C-N	6.54	126.31	119.05
1	C	516	THR	C-N-CA	6.54	126.31	119.05
1	C	32	GLU	CB-CG-CD	6.53	123.70	112.60
1	D	575	PRO	O-C-N	6.53	124.31	121.31
1	A	712	ASP	CA-C-O	6.53	125.91	118.47
1	D	636	ARG	CA-C-O	-6.53	114.46	121.38
1	A	272	PHE	CA-C-O	-6.51	112.53	120.54
1	A	751	ILE	CA-C-O	6.50	126.06	119.82
1	C	236	HIS	CA-C-N	6.50	129.31	120.54
1	C	236	HIS	C-N-CA	6.50	129.31	120.54
1	B	593	ILE	CA-C-N	6.45	127.90	119.84
1	B	593	ILE	C-N-CA	6.45	127.90	119.84
1	D	155	ASP	CA-C-N	6.44	126.13	119.82
1	D	155	ASP	C-N-CA	6.44	126.13	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	728	PHE	CA-CB-CG	6.44	120.24	113.80
1	B	629	HIS	CA-CB-CG	-6.44	107.36	113.80
1	A	392	HIS	CA-C-N	6.43	126.55	119.87
1	A	392	HIS	C-N-CA	6.43	126.55	119.87
1	C	271	GLY	O-C-N	-6.42	118.03	123.23
1	C	503	GLU	CA-C-O	-6.42	112.38	120.28
1	B	210	ASP	CA-CB-CG	6.42	119.02	112.60
1	B	567	THR	CA-C-N	6.42	131.39	121.19
1	B	567	THR	C-N-CA	6.42	131.39	121.19
1	B	641	THR	CA-C-O	-6.40	113.45	120.30
1	D	368	GLN	CB-CG-CD	6.39	123.47	112.60
1	C	442	ASN	CA-C-N	-6.38	112.53	122.67
1	C	442	ASN	C-N-CA	-6.38	112.53	122.67
1	A	386	ASN	OD1-CG-ND2	-6.37	116.23	122.60
1	C	476	GLY	CA-C-N	6.36	125.94	119.19
1	C	476	GLY	C-N-CA	6.36	125.94	119.19
1	B	585	ASP	CA-C-N	6.36	126.28	119.28
1	B	585	ASP	C-N-CA	6.36	126.28	119.28
1	B	409	GLN	CA-C-N	6.35	126.99	120.00
1	B	409	GLN	C-N-CA	6.35	126.99	120.00
1	C	237	ASP	N-CA-C	6.35	118.73	111.11
1	C	292	HIS	CA-CB-CG	6.33	120.14	113.80
1	D	302	LEU	CA-C-O	-6.33	115.36	122.01
1	B	171	GLY	N-CA-C	6.32	119.29	112.33
1	D	61	ARG	NE-CZ-NH1	-6.30	115.19	121.50
1	D	648	LEU	CA-C-N	6.30	127.25	120.13
1	D	648	LEU	C-N-CA	6.30	127.25	120.13
1	D	37	ARG	CA-C-O	6.29	125.38	119.59
1	D	431	ILE	N-CA-C	-6.29	102.79	108.95
1	B	264	ARG	CA-C-O	6.28	127.19	119.97
1	D	405	ASP	CA-CB-CG	6.28	118.88	112.60
1	B	449	HIS	CA-CB-CG	6.27	120.07	113.80
1	C	639	GLU	CA-C-O	-6.27	114.52	121.23
1	C	72	ARG	CA-C-O	-6.26	114.15	121.16
1	D	80	LEU	CA-C-O	-6.25	113.62	120.81
1	A	740	ARG	NE-CZ-NH2	6.24	124.81	119.20
1	D	608	ASN	CA-CB-CG	6.24	118.84	112.60
1	C	168	THR	N-CA-C	-6.22	101.00	110.14
1	A	479	ARG	CD-NE-CZ	6.20	133.09	124.40
1	D	135	HIS	CA-CB-CG	6.20	120.00	113.80
1	B	101	GLY	CA-C-N	6.20	126.11	119.85
1	B	101	GLY	C-N-CA	6.20	126.11	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	574	THR	CA-C-O	6.20	125.28	119.76
1	A	431	ILE	CA-C-N	6.19	127.58	119.84
1	A	431	ILE	C-N-CA	6.19	127.58	119.84
1	B	271	GLY	O-C-N	-6.19	117.92	123.37
1	C	159	ILE	CB-CA-C	6.18	120.04	110.83
1	D	675	ILE	CA-C-O	6.18	124.75	119.38
1	D	246	GLN	CA-C-N	6.14	125.84	119.82
1	D	246	GLN	C-N-CA	6.14	125.84	119.82
1	D	182	ILE	N-CA-C	-6.14	101.08	109.55
1	D	303	VAL	CA-C-O	-6.13	114.75	121.92
1	C	342	PRO	N-CA-CB	6.12	109.02	103.33
1	C	339	GLN	N-CA-C	-6.11	98.77	108.73
1	C	167	SER	N-CA-C	6.10	116.62	108.38
1	C	742	TRP	CA-C-N	6.10	130.36	120.60
1	C	742	TRP	C-N-CA	6.10	130.36	120.60
1	B	284	GLY	N-CA-C	-6.09	106.75	115.64
1	B	392	HIS	CA-C-N	6.09	125.98	119.28
1	B	392	HIS	C-N-CA	6.09	125.98	119.28
1	B	405	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	476	GLY	CA-C-N	6.09	125.64	119.19
1	A	476	GLY	C-N-CA	6.09	125.64	119.19
1	B	224	GLU	CB-CA-C	6.07	119.11	109.52
1	A	194	GLY	CA-C-O	-6.07	117.42	122.33
1	B	349	PHE	CA-CB-CG	-6.07	107.73	113.80
1	A	387	GLU	CA-C-O	-6.06	114.12	120.55
1	C	159	ILE	CA-CB-CG2	6.06	120.80	110.50
1	D	278	ARG	NE-CZ-NH1	-6.05	115.45	121.50
1	D	28	SER	N-CA-CB	6.05	120.71	110.49
1	D	281	ASN	CA-CB-CG	6.05	118.65	112.60
1	D	44	PRO	O-C-N	6.04	123.99	121.15
1	D	45	PRO	N-CA-CB	6.03	109.59	103.25
1	D	171	GLY	N-CA-C	6.03	118.97	112.33
1	D	37	ARG	N-CA-CB	-6.03	99.80	110.05
1	A	389	ALA	CA-C-O	-6.03	114.52	121.15
1	B	615	ASP	N-CA-C	-6.03	103.36	112.04
1	B	123	PRO	N-CA-CB	6.02	108.66	103.36
1	A	381	ASN	CA-CB-CG	-6.01	106.59	112.60
1	C	314	ASP	CA-C-N	6.00	125.70	119.82
1	C	314	ASP	C-N-CA	6.00	125.70	119.82
1	C	742	TRP	O-C-N	-5.98	115.78	122.12
1	D	466	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	B	643	ASP	CA-CB-CG	5.96	118.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	GLU	CA-C-O	5.95	127.07	120.82
1	C	33	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	486	GLN	CB-CG-CD	5.94	122.70	112.60
1	B	44	PRO	N-CA-CB	5.92	108.83	103.08
1	C	551	ASP	CA-CB-CG	-5.92	106.68	112.60
1	A	483	GLU	CA-C-O	-5.92	113.75	120.32
1	D	100	ARG	CD-NE-CZ	5.92	132.68	124.40
1	D	413	PHE	CA-C-N	5.91	128.20	120.28
1	D	413	PHE	C-N-CA	5.91	128.20	120.28
1	A	414	SER	CA-C-O	-5.91	114.16	120.42
1	B	425	GLY	CA-C-N	5.91	126.42	120.04
1	B	425	GLY	C-N-CA	5.91	126.42	120.04
1	A	636	ARG	CA-C-O	-5.89	114.93	121.23
1	D	294	LYS	CA-C-O	5.88	126.97	119.67
1	C	447	GLY	CA-C-O	-5.88	117.29	121.88
1	A	236	HIS	CA-CB-CG	5.86	119.66	113.80
1	D	214	PHE	CA-C-N	5.86	125.55	119.05
1	D	214	PHE	C-N-CA	5.86	125.55	119.05
1	C	98	GLY	N-CA-C	-5.84	105.41	112.48
1	B	283	GLU	CB-CG-CD	5.84	122.53	112.60
1	C	580	ASN	CA-CB-CG	-5.84	106.76	112.60
1	B	203	THR	CA-C-N	5.83	126.59	120.12
1	B	203	THR	C-N-CA	5.83	126.59	120.12
1	B	37	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	C	339	GLN	CA-C-O	-5.81	114.14	120.36
1	B	516	THR	CA-C-N	5.80	125.49	119.05
1	B	516	THR	C-N-CA	5.80	125.49	119.05
1	B	648	LEU	CA-C-N	5.80	125.56	119.76
1	B	648	LEU	C-N-CA	5.80	125.56	119.76
1	D	247	PRO	N-CA-CB	5.80	109.03	103.52
1	D	292	HIS	CA-CB-CG	5.80	119.60	113.80
1	C	140	PRO	N-CA-CB	5.79	108.71	103.33
1	B	182	ILE	N-CA-C	-5.78	99.99	109.12
1	B	569	ASP	CA-CB-CG	5.78	118.38	112.60
1	B	667	VAL	CA-C-N	5.77	125.75	120.03
1	B	667	VAL	C-N-CA	5.77	125.75	120.03
1	D	210	ASP	CA-C-O	5.77	126.59	120.36
1	C	214	PHE	CA-CB-CG	-5.77	108.03	113.80
1	D	457	PRO	N-CA-CB	5.76	109.24	103.48
1	C	206	PHE	CA-CB-CG	-5.76	108.04	113.80
1	D	32	GLU	CB-CG-CD	5.75	122.37	112.60
1	B	38	PRO	N-CA-CB	5.74	108.41	103.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ARG	NE-CZ-NH2	-5.74	114.03	119.20
1	D	598	VAL	N-CA-CB	-5.74	98.77	111.50
1	D	224	GLU	CA-C-O	5.74	126.13	120.17
1	D	166	PHE	CA-C-O	-5.73	114.67	121.66
1	C	50	THR	CA-C-O	-5.73	115.22	121.87
1	C	161	PRO	N-CA-CB	5.72	108.66	103.34
1	B	565	GLU	CA-C-O	-5.72	114.24	120.36
1	C	93	ASN	N-CA-C	5.72	118.09	109.23
1	C	326	ILE	CA-C-N	5.71	128.98	120.31
1	C	326	ILE	C-N-CA	5.71	128.98	120.31
1	A	437	THR	N-CA-C	-5.69	106.38	113.38
1	B	728	PHE	CA-CB-CG	5.69	119.49	113.80
1	A	527	PHE	CA-C-O	-5.69	114.84	120.82
1	A	146	ASP	CA-CB-CG	5.68	118.28	112.60
1	D	751	ILE	CA-C-O	5.68	127.56	119.95
1	B	234	SER	N-CA-C	-5.67	106.41	113.38
1	C	263	PRO	N-CA-CB	5.67	108.36	103.31
1	C	445	ARG	NE-CZ-NH2	-5.66	114.10	119.20
1	C	509	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	B	52	PRO	CA-C-N	5.66	126.37	120.03
1	B	52	PRO	C-N-CA	5.66	126.37	120.03
1	B	405	ASP	CA-C-N	5.66	125.27	119.56
1	B	405	ASP	C-N-CA	5.66	125.27	119.56
1	A	612	ARG	CD-NE-CZ	5.65	132.31	124.40
1	B	649	PRO	N-CA-CB	5.64	108.59	103.34
1	D	419	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	C	498	SER	CA-C-N	5.64	125.75	119.32
1	C	498	SER	C-N-CA	5.64	125.75	119.32
1	D	612	ARG	CG-CD-NE	5.63	124.39	112.00
1	A	507	HIS	CA-C-N	5.63	125.74	119.32
1	A	507	HIS	C-N-CA	5.63	125.74	119.32
1	D	638	GLY	O-C-N	-5.63	119.42	123.08
1	B	45	PRO	N-CA-CB	5.63	108.26	103.19
1	A	542	ARG	NE-CZ-NH2	-5.63	114.13	119.20
1	B	27	ASP	CA-C-O	5.62	130.36	120.80
1	D	476	GLY	CA-C-N	5.62	125.15	119.19
1	D	476	GLY	C-N-CA	5.62	125.15	119.19
1	A	418	THR	CA-C-N	5.61	128.36	120.28
1	A	418	THR	C-N-CA	5.61	128.36	120.28
1	B	147	ILE	CA-C-O	-5.61	113.82	119.20
1	A	585	ASP	CA-C-N	5.60	125.27	119.56
1	A	585	ASP	C-N-CA	5.60	125.27	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	ARG	CD-NE-CZ	5.60	132.24	124.40
1	B	37	ARG	CA-C-N	5.60	125.78	119.90
1	B	37	ARG	C-N-CA	5.60	125.78	119.90
1	A	49	PRO	CA-C-O	-5.59	114.96	121.34
1	A	693	LYS	CA-C-N	5.59	125.52	119.76
1	A	693	LYS	C-N-CA	5.59	125.52	119.76
1	B	349	PHE	CA-C-N	-5.59	113.72	122.73
1	B	349	PHE	C-N-CA	-5.59	113.72	122.73
1	B	120	GLU	N-CA-C	5.59	117.38	111.28
1	B	60	THR	N-CA-C	-5.59	99.41	108.41
1	B	435	ARG	CB-CA-C	-5.57	100.42	109.56
1	A	535	VAL	CA-C-O	-5.57	115.16	120.95
1	C	334	TYR	CA-C-O	5.57	127.12	120.28
1	C	212	HIS	CA-CB-CG	-5.56	108.24	113.80
1	D	41	GLU	CB-CG-CD	5.55	122.04	112.60
1	D	41	GLU	CA-CB-CG	5.55	125.20	114.10
1	C	341	ILE	CB-CA-C	-5.54	104.75	110.13
1	A	667	VAL	CA-C-N	5.54	126.01	120.52
1	A	667	VAL	C-N-CA	5.54	126.01	120.52
1	B	57	ALA	CA-C-N	5.54	125.37	119.28
1	B	57	ALA	C-N-CA	5.54	125.37	119.28
1	C	486	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	B	342	PRO	N-CA-CB	5.53	108.16	103.35
1	B	250	LEU	N-CA-C	5.52	117.30	111.28
1	D	593	ILE	CA-C-N	5.52	126.75	119.84
1	D	593	ILE	C-N-CA	5.52	126.75	119.84
1	C	468	ASN	CA-C-O	-5.52	112.36	119.59
1	B	41	GLU	CB-CG-CD	5.51	121.97	112.60
1	B	55	LEU	N-CA-C	-5.51	105.68	112.90
1	B	379	PRO	CB-CA-C	-5.51	102.92	111.40
1	C	648	LEU	CA-C-N	5.51	126.73	119.84
1	C	648	LEU	C-N-CA	5.51	126.73	119.84
1	A	750	LYS	N-CA-C	-5.51	105.69	112.90
1	B	161	PRO	N-CA-CB	5.51	108.14	103.35
1	B	263	PRO	N-CA-CB	5.51	108.14	103.35
1	B	431	ILE	CA-C-N	5.50	126.72	119.84
1	B	431	ILE	C-N-CA	5.50	126.72	119.84
1	D	326	ILE	O-C-N	-5.50	116.53	121.87
1	D	438	CYS	CA-C-N	5.50	125.45	119.78
1	D	438	CYS	C-N-CA	5.50	125.45	119.78
1	B	471	ARG	N-CA-C	5.50	118.45	109.59
1	B	271	GLY	CA-C-O	5.50	126.35	121.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	ILE	CB-CG1-CD1	-5.49	102.26	113.80
1	A	317	PHE	N-CA-C	5.48	117.25	111.28
1	B	290	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	A	214	PHE	CA-C-N	5.48	125.56	119.32
1	A	214	PHE	C-N-CA	5.48	125.56	119.32
1	B	498	SER	CA-C-N	5.47	125.13	119.05
1	B	498	SER	C-N-CA	5.47	125.13	119.05
1	D	341	ILE	CA-C-N	5.47	125.39	119.76
1	D	341	ILE	C-N-CA	5.47	125.39	119.76
1	A	197	ASP	CA-CB-CG	5.47	118.07	112.60
1	C	657	ALA	CA-C-N	5.46	125.43	120.03
1	C	657	ALA	C-N-CA	5.46	125.43	120.03
1	C	319	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	B	237	ASP	CA-C-O	-5.44	114.65	121.02
1	A	471	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	D	392	HIS	CA-C-N	5.44	125.05	119.56
1	D	392	HIS	C-N-CA	5.44	125.05	119.56
1	A	214	PHE	CA-CB-CG	-5.44	108.36	113.80
1	B	48	GLN	OE1-CD-NE2	5.43	128.03	122.60
1	B	615	ASP	CA-CB-CG	5.43	118.03	112.60
1	B	133	ALA	N-CA-C	5.43	118.08	109.50
1	D	304	TRP	N-CA-C	5.43	117.62	111.11
1	D	477	PRO	N-CA-CB	5.43	109.28	103.52
1	A	306	GLU	CA-C-N	5.42	127.48	120.44
1	A	306	GLU	C-N-CA	5.42	127.48	120.44
1	C	507	HIS	CA-C-N	5.42	125.50	119.32
1	C	507	HIS	C-N-CA	5.42	125.50	119.32
1	D	70	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	498	SER	CA-C-O	5.41	124.84	119.75
1	D	319	ARG	CD-NE-CZ	5.41	131.98	124.40
1	C	702	ARG	CA-C-N	5.41	128.07	120.28
1	C	702	ARG	C-N-CA	5.41	128.07	120.28
1	A	421	SER	N-CA-C	-5.40	106.37	113.12
1	B	428	PHE	CA-CB-CG	-5.40	108.40	113.80
1	B	355	ASP	CA-C-N	5.40	125.48	119.87
1	B	355	ASP	C-N-CA	5.40	125.48	119.87
1	C	392	HIS	CA-C-N	5.39	125.48	119.87
1	C	392	HIS	C-N-CA	5.39	125.48	119.87
1	A	71	VAL	CA-C-O	-5.38	113.70	119.35
1	B	53	GLY	N-CA-C	5.38	119.39	112.83
1	C	157	ASN	OD1-CG-ND2	5.38	127.98	122.60
1	D	143	SER	CA-C-O	-5.38	115.13	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	342	PRO	N-CA-CB	5.38	108.10	103.31
1	B	435	ARG	N-CA-C	5.38	115.78	109.60
1	C	752	PRO	N-CA-CB	5.37	106.30	102.65
1	A	361	PRO	N-CA-CB	5.37	108.02	103.19
1	D	712	ASP	CA-C-O	5.37	126.45	120.82
1	C	496	GLU	N-CA-CB	-5.36	101.55	111.52
1	B	719	VAL	N-CA-CB	5.35	116.55	110.72
1	B	466	ASN	CA-CB-CG	-5.35	107.25	112.60
1	D	609	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	225	PRO	N-CA-C	5.35	121.56	113.81
1	D	674	ASP	CA-C-O	-5.35	114.86	120.63
1	D	170[A]	GLN	N-CA-C	5.34	117.92	111.40
1	D	170[B]	GLN	N-CA-C	5.34	117.92	111.40
1	D	250	LEU	N-CA-C	5.33	117.09	111.28
1	D	291	PHE	O-C-N	-5.33	116.98	123.16
1	A	194	GLY	O-C-N	5.32	127.95	123.43
1	A	272	PHE	CA-CB-CG	5.32	119.12	113.80
1	C	431	ILE	N-CA-C	-5.32	103.74	108.95
1	A	745	ILE	CA-C-N	5.32	125.38	119.32
1	A	745	ILE	C-N-CA	5.32	125.38	119.32
1	A	386	ASN	CB-CG-ND2	5.31	124.37	116.40
1	D	31	PRO	N-CA-CB	5.31	108.04	103.31
1	A	290	ARG	CD-NE-CZ	-5.31	116.97	124.40
1	C	121	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	A	579	VAL	CA-C-O	-5.30	114.66	120.97
1	D	237	ASP	CA-C-O	-5.30	115.23	120.90
1	C	304	TRP	N-CA-C	5.29	117.47	111.02
1	D	551	ASP	CA-C-O	5.29	128.07	120.51
1	A	224	GLU	CA-C-N	5.29	125.60	119.47
1	A	224	GLU	C-N-CA	5.29	125.60	119.47
1	C	407	LEU	CA-C-O	5.29	126.20	120.55
1	B	225	PRO	N-CA-C	5.28	120.49	113.57
1	B	311	THR	N-CA-CB	5.28	118.35	110.22
1	C	486	GLN	CB-CG-CD	5.28	121.58	112.60
1	B	636	ARG	CA-C-O	-5.27	115.81	121.45
1	A	501	PHE	N-CA-C	-5.27	106.85	113.28
1	A	580	ASN	CA-CB-CG	-5.27	107.33	112.60
1	C	434	ASN	CA-C-O	-5.27	112.78	119.31
1	D	586	PRO	N-CA-CB	5.26	108.74	103.48
1	B	283	GLU	N-CA-CB	5.25	118.42	110.28
1	A	38	PRO	CB-CA-C	-5.25	104.69	111.46
1	D	123	PRO	CA-C-O	-5.25	115.36	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	366	PRO	N-CA-CB	5.24	108.32	103.39
1	C	203	THR	CA-C-N	5.24	124.85	119.56
1	C	203	THR	C-N-CA	5.24	124.85	119.56
1	D	38	PRO	CA-C-O	5.24	127.31	121.34
1	C	168	THR	N-CA-CB	5.23	118.49	110.70
1	B	166	PHE	CA-C-O	-5.23	115.25	121.16
1	C	615	ASP	N-CA-C	-5.22	105.50	111.14
1	B	246	GLN	CA-C-N	5.22	125.30	119.87
1	B	246	GLN	C-N-CA	5.22	125.30	119.87
1	B	370	VAL	N-CA-CB	-5.22	105.08	112.12
1	D	366	PRO	N-CA-CB	5.22	108.30	103.39
1	D	712	ASP	CA-C-N	5.22	127.79	120.28
1	D	712	ASP	C-N-CA	5.22	127.79	120.28
1	A	356	PRO	N-CA-CB	5.21	108.56	102.88
1	C	709	LYS	CA-CB-CG	5.21	124.53	114.10
1	D	745	ILE	CA-C-N	5.21	125.27	119.32
1	D	745	ILE	C-N-CA	5.21	125.27	119.32
1	A	288	PHE	CA-C-O	-5.21	115.32	121.16
1	B	366	PRO	N-CA-CB	5.21	108.17	103.33
1	A	133	ALA	N-CA-C	5.21	117.78	109.81
1	D	133	ALA	N-CA-C	5.21	117.33	109.41
1	A	350	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	572	ASN	N-CA-C	5.20	119.72	113.17
1	B	461	GLU	CB-CG-CD	5.20	121.43	112.60
1	D	585	ASP	CA-C-N	5.20	124.86	119.56
1	D	585	ASP	C-N-CA	5.20	124.86	119.56
1	D	713	GLN	N-CA-CB	-5.20	102.22	110.22
1	C	330	ASP	CB-CA-C	-5.19	103.64	112.00
1	C	540	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	B	320	ARG	CA-C-O	5.19	126.27	120.82
1	D	72	ARG	NE-CZ-NH2	-5.18	114.53	119.20
1	D	649	PRO	N-CA-CB	5.18	107.66	103.36
1	B	340	LEU	CA-C-N	5.18	127.36	122.85
1	B	340	LEU	C-N-CA	5.18	127.36	122.85
1	A	710	ILE	CA-C-O	5.18	127.25	120.78
1	B	375	LEU	CA-C-O	-5.18	115.04	120.58
1	C	466	ASN	CA-CB-CG	-5.18	107.42	112.60
1	A	166	PHE	CA-C-O	-5.18	115.22	120.71
1	A	498	SER	CA-C-N	5.18	125.47	119.47
1	A	498	SER	C-N-CA	5.18	125.47	119.47
1	A	60	THR	CA-C-O	-5.17	114.75	120.60
1	D	320	ARG	NE-CZ-NH2	-5.17	114.54	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	526	GLY	N-CA-C	-5.17	106.50	112.50
1	D	555	ALA	CA-C-N	5.17	127.16	120.44
1	D	555	ALA	C-N-CA	5.17	127.16	120.44
1	C	536	ARG	CA-C-N	5.17	124.97	119.28
1	C	536	ARG	C-N-CA	5.17	124.97	119.28
1	D	585	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	682	ASN	CA-CB-CG	-5.17	107.43	112.60
1	D	691	HIS	CA-C-N	5.17	129.89	122.40
1	D	691	HIS	C-N-CA	5.17	129.89	122.40
1	C	319	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	A	280	ILE	CA-C-O	-5.16	115.02	120.39
1	C	659	SER	CA-C-N	5.16	127.45	120.38
1	C	659	SER	C-N-CA	5.16	127.45	120.38
1	B	275	HIS	CB-CA-C	-5.16	99.50	109.76
1	B	560	LYS	CA-C-O	-5.16	115.08	120.55
1	A	433	ILE	CA-C-O	-5.15	115.06	120.57
1	C	278	ARG	O-C-N	5.15	129.58	123.24
1	A	450	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	D	51	ALA	N-CA-CB	-5.15	104.81	111.35
1	D	57	ALA	CA-C-N	5.15	124.94	119.28
1	D	57	ALA	C-N-CA	5.15	124.94	119.28
1	B	323	TRP	CA-C-N	5.14	128.13	120.31
1	B	323	TRP	C-N-CA	5.14	128.13	120.31
1	C	234	SER	N-CA-C	-5.14	107.00	113.28
1	C	246	GLN	CA-C-N	5.14	124.80	119.56
1	C	246	GLN	C-N-CA	5.14	124.80	119.56
1	C	96	ARG	CA-C-O	5.14	127.26	121.51
1	B	374	VAL	CA-C-O	-5.13	115.00	120.39
1	D	37	ARG	N-CA-C	5.13	118.91	109.10
1	C	333	GLU	CA-C-O	5.13	126.24	120.70
1	A	262	ILE	CA-C-N	5.12	125.03	119.85
1	A	262	ILE	C-N-CA	5.12	125.03	119.85
1	C	43	THR	CA-C-N	5.12	125.66	120.38
1	C	43	THR	C-N-CA	5.12	125.66	120.38
1	B	609	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	338	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	37	ARG	CA-C-N	5.11	125.03	119.76
1	A	37	ARG	C-N-CA	5.11	125.03	119.76
1	C	30	ALA	CA-C-N	5.11	125.01	119.85
1	C	30	ALA	C-N-CA	5.11	125.01	119.85
1	C	49	PRO	N-CA-C	-5.11	103.17	111.14
1	A	377	ARG	NH1-CZ-NH2	5.11	125.94	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	556	GLN	CB-CA-C	-5.11	102.17	110.85
1	A	273	GLY	CA-C-N	5.10	131.15	121.97
1	A	273	GLY	C-N-CA	5.10	131.15	121.97
1	D	463	ASN	OD1-CG-ND2	5.10	127.70	122.60
1	D	693	LYS	CA-C-N	5.10	125.01	119.76
1	D	693	LYS	C-N-CA	5.10	125.01	119.76
1	D	709	LYS	CA-CB-CG	5.10	124.30	114.10
1	D	405	ASP	CA-C-N	5.10	124.71	119.56
1	D	405	ASP	C-N-CA	5.10	124.71	119.56
1	A	506	SER	CA-C-N	5.09	127.09	120.26
1	A	506	SER	C-N-CA	5.09	127.09	120.26
1	D	474	PRO	CA-C-O	5.09	124.75	120.73
1	A	37	ARG	CD-NE-CZ	5.09	131.53	124.40
1	B	369	ARG	CA-C-O	-5.09	114.68	120.58
1	B	135	HIS	CA-CB-CG	5.08	118.89	113.80
1	C	454	ASP	CA-CB-CG	-5.08	107.52	112.60
1	B	574	THR	CA-C-N	5.07	125.61	120.38
1	B	574	THR	C-N-CA	5.07	125.61	120.38
1	C	471	ARG	N-CA-C	5.07	118.33	110.17
1	D	30	ALA	CA-C-N	5.07	124.98	119.76
1	D	30	ALA	C-N-CA	5.07	124.98	119.76
1	C	424	GLY	N-CA-C	5.07	122.60	115.30
1	C	733	LEU	CA-C-O	5.05	125.78	119.97
1	B	557	ALA	N-CA-C	-5.05	105.86	111.36
1	B	403	THR	N-CA-CB	5.05	119.74	111.31
1	B	551	ASP	CA-C-N	5.04	127.45	120.29
1	B	551	ASP	C-N-CA	5.04	127.45	120.29
1	A	361	PRO	CA-C-N	5.04	127.53	120.28
1	A	361	PRO	C-N-CA	5.04	127.53	120.28
1	D	125	ARG	CA-C-O	-5.04	115.65	121.19
1	B	265	SER	N-CA-CB	-5.03	103.92	111.56
1	D	180	ARG	CD-NE-CZ	5.02	131.43	124.40
1	A	577	PRO	CB-CA-C	-5.02	104.38	110.95
1	A	648	LEU	CA-C-O	5.02	123.57	119.36
1	C	540	ARG	CA-C-O	5.01	125.73	120.42
1	C	574	THR	CA-C-N	5.01	123.27	119.66
1	C	574	THR	C-N-CA	5.01	123.27	119.66
1	D	210	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	271	GLY	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5747	0	5583	109	1
1	B	5747	0	5583	134	1
1	C	5747	0	5583	107	0
1	D	5747	0	5583	126	0
2	A	43	0	30	6	0
2	B	43	0	30	1	0
2	C	43	0	30	3	0
2	D	43	0	30	2	0
3	A	732	0	0	8	0
3	B	641	0	0	19	0
3	C	673	0	0	12	0
3	D	721	0	0	7	0
All	All	25927	0	22452	442	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (442) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:MET:HE2	1:C:451:MET:HE2	1.35	1.06
1:B:451:MET:HE2	1:D:451:MET:HE2	1.49	0.93
1:D:750:LYS:HZ2	1:D:751:ILE:H	1.15	0.91
1:C:392:HIS:ND1	1:C:415:TYR:HB2	1.97	0.80
1:A:51:ALA:HB1	1:A:52:PRO:HD2	1.66	0.76
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.66	0.75
1:C:748:ILE:O	1:C:751:ILE:HG22	1.84	0.75
1:D:750:LYS:HZ2	1:D:751:ILE:N	1.84	0.75
1:D:392:HIS:ND1	1:D:415:TYR:HB2	2.02	0.75
1:A:392:HIS:ND1	1:A:415:TYR:HB2	2.02	0.74
1:C:28:SER:HA	3:C:3649:HOH:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.69	0.74
1:D:750:LYS:NZ	1:D:751:ILE:H	1.86	0.73
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.70	0.73
1:D:333:GLU:HG2	1:D:374:VAL:HG22	1.70	0.72
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.73	0.71
1:B:36:HIS:CD2	1:B:37:ARG:HD3	2.26	0.70
1:A:71:VAL:HG23	1:C:453:ILE:HD12	1.74	0.70
1:B:392:HIS:ND1	1:B:415:TYR:HB2	2.07	0.69
1:B:222:LYS:HB3	1:B:223:PRO:CD	2.23	0.67
1:B:521:ARG:HH21	1:B:745:ILE:HD13	1.59	0.67
1:A:214:PHE:HB3	1:A:215:PRO:HD3	1.77	0.67
1:A:637:MET:HG3	1:D:532:SER:HB2	1.77	0.67
1:A:170[B]:GLN:HG3	1:A:232:GLY:HA2	1.78	0.66
1:B:583:LYS:O	1:B:584:LYS:HB3	1.96	0.65
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.79	0.65
1:A:490:GLU:HG2	1:B:490:GLU:HG2	1.79	0.65
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.27	0.65
1:B:222:LYS:HB3	1:B:223:PRO:HD2	1.77	0.65
1:A:274:ILE:HD12	2:A:760:HEM:HBB2	1.78	0.64
1:A:565:GLU:HG3	3:A:2882:HOH:O	1.96	0.64
1:B:509:ARG:HD2	1:B:576:PRO:HD2	1.80	0.64
1:B:468:ASN:HD22	1:D:27:ASP:N	1.95	0.64
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.80	0.64
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.13	0.63
1:C:260:ARG:HD3	1:C:590:LEU:HD21	1.80	0.63
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.12	0.63
1:B:507:HIS:N	1:B:508:PRO:HD2	2.14	0.63
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.79	0.62
1:C:438:CYS:HB2	1:C:439:PRO:HD2	1.81	0.62
1:C:610:GLU:OE1	1:C:643:ASP:HA	2.00	0.62
1:A:708:ILE:O	1:A:710:ILE:HG22	1.98	0.62
1:D:170[B]:GLN:HG3	1:D:232:GLY:HA2	1.81	0.62
1:B:606:LEU:HB2	1:B:667:VAL:HG22	1.82	0.62
1:C:435:ARG:HD3	3:C:2182:HOH:O	1.99	0.62
1:B:596:GLY:HA3	3:B:3195:HOH:O	2.00	0.61
1:D:122:ILE:HB	1:D:123:PRO:HD2	1.81	0.61
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.35	0.61
1:C:310:LEU:HD13	1:C:660:LEU:HB3	1.82	0.61
1:D:629:HIS:HD2	3:D:2554:HOH:O	1.83	0.60
1:C:578:ASP:HB2	1:C:582:LEU:O	2.00	0.60
1:C:507:HIS:N	1:C:508:PRO:HD2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:617:LEU:HD12	3:C:3230:HOH:O	2.02	0.60
1:D:689:TYR:HA	1:D:744:ARG:NH1	2.17	0.60
1:D:459:ASN:HD22	1:D:459:ASN:H	1.49	0.60
3:B:1354:HOH:O	1:D:193:GLU:HG2	2.02	0.60
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	1.84	0.59
1:D:359:LEU:H	1:D:507:HIS:CD2	2.20	0.59
1:C:704:PHE:O	1:C:707:THR:HG22	2.02	0.59
1:C:359:LEU:C	1:C:359:LEU:HD12	2.28	0.59
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.33	0.59
1:B:583:LYS:H	1:B:583:LYS:CE	2.15	0.59
1:A:36:HIS:CD2	1:A:36:HIS:H	2.20	0.58
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.38	0.58
1:C:751:ILE:HB	3:C:3367:HOH:O	2.03	0.58
1:B:640:VAL:HG13	1:B:650:ILE:HD11	1.85	0.58
1:D:65:LEU:HD21	1:D:135:HIS:CG	2.38	0.58
1:B:321:GLU:HG3	3:B:2921:HOH:O	2.02	0.58
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.86	0.57
1:D:744:ARG:HA	1:D:747:LYS:HD3	1.85	0.57
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.86	0.57
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.87	0.57
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.40	0.57
1:B:552:LEU:O	1:B:552:LEU:HD22	2.05	0.56
1:B:604:ALA:HB1	1:B:633:LEU:HD22	1.87	0.56
1:D:640:VAL:HG13	1:D:650:ILE:HD11	1.87	0.56
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.36	0.56
1:B:155:ASP:OD1	3:B:4138:HOH:O	2.17	0.56
1:D:535:VAL:O	1:D:537:PRO:HD3	2.05	0.56
1:A:28:SER:HB2	1:D:245:LEU:HD22	1.88	0.56
1:B:719:VAL:HG13	1:B:731:GLU:OE2	2.05	0.56
1:D:516:THR:HB	1:D:517:PRO:HD2	1.88	0.56
1:D:533:LYS:NZ	3:D:3941:HOH:O	2.38	0.56
1:C:535:VAL:O	1:C:537:PRO:HD3	2.06	0.56
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.41	0.56
1:D:516:THR:HB	1:D:517:PRO:CD	2.36	0.56
1:D:700:ASP:HB3	1:D:703:LYS:HE2	1.88	0.56
1:B:556:GLN:HG2	1:B:566:LEU:HD23	1.88	0.55
1:C:205:ILE:HD13	1:C:205:ILE:H	1.72	0.55
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.21	0.55
1:A:438:CYS:HB2	1:A:439:PRO:CD	2.37	0.55
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.89	0.55
1:D:144:LEU:HD12	1:D:153:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:LEU:HD11	1:D:370:VAL:HG13	1.89	0.55
1:D:392:HIS:CE1	1:D:415:TYR:HB2	2.41	0.55
1:A:404:ASN:O	1:A:405:ASP:C	2.48	0.55
1:A:469:TRP:CE3	1:A:471:ARG:HG3	2.42	0.55
1:A:748:ILE:O	1:A:751:ILE:HG13	2.07	0.55
1:B:231:GLN:HB2	3:C:1859:HOH:O	2.07	0.55
1:B:745:ILE:O	1:B:748:ILE:HG12	2.07	0.54
1:D:692:LEU:HB2	1:D:740:ARG:HB3	1.89	0.54
1:A:126:ILE:CD1	1:D:120:GLU:HB2	2.37	0.54
1:B:364:LEU:HD11	1:B:580:ASN:HB2	1.89	0.54
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.72	0.54
1:A:294:LYS:NZ	3:A:2213:HOH:O	2.40	0.54
1:B:27:ASP:OD2	1:D:468:ASN:ND2	2.37	0.54
1:B:477:PRO:HD2	3:B:1270:HOH:O	2.06	0.54
1:C:51:ALA:HB1	1:C:52:PRO:HD2	1.89	0.54
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.16	0.54
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.89	0.54
1:C:170[B]:GLN:HG3	1:C:232:GLY:HA2	1.90	0.54
1:B:583:LYS:H	1:B:583:LYS:NZ	2.05	0.54
1:D:750:LYS:CD	1:D:751:ILE:H	2.21	0.54
1:D:267:ARG:HG3	3:D:2920:HOH:O	2.08	0.54
2:A:760:HEM:HBB2	2:A:760:HEM:HMB1	1.89	0.53
1:B:344:GLU:CD	1:B:344:GLU:H	2.14	0.53
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.38	0.53
1:B:634:TYR:O	1:B:653:THR:HA	2.07	0.53
1:C:193:GLU:OE1	1:C:479:ARG:HD3	2.08	0.53
2:C:760:HEM:CMC	2:C:760:HEM:HBC2	2.38	0.53
1:B:207:PHE:O	1:B:249:THR:HA	2.09	0.53
1:B:669:CYS:SG	1:B:670:GLY:N	2.80	0.53
1:C:404:ASN:O	1:C:405:ASP:C	2.49	0.53
1:B:274:ILE:HD12	2:B:760:HEM:HMB1	1.91	0.52
1:D:397:VAL:HB	1:D:398:PRO:HD2	1.91	0.52
1:B:213:LYS:HD3	1:C:92:GLN:HA	1.91	0.52
1:B:556:GLN:HA	1:B:566:LEU:HD21	1.90	0.52
2:C:760:HEM:HBC2	2:C:760:HEM:HMC1	1.91	0.52
1:A:369:ARG:HG2	1:A:369:ARG:HH21	1.75	0.52
1:D:745:ILE:HB	1:D:746:PRO:HD3	1.90	0.52
1:A:51:ALA:HB1	1:A:52:PRO:CD	2.37	0.52
1:B:521:ARG:NH2	1:B:745:ILE:HG21	2.24	0.52
1:A:351:PHE:HB2	1:A:358:LYS:HG3	1.91	0.52
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:HIS:ND1	1:A:393:PRO:HD2	2.25	0.52
1:B:612:ARG:HD2	1:B:670:GLY:HA2	1.92	0.52
1:A:468:ASN:O	1:A:471:ARG:HG2	2.10	0.52
1:C:629:HIS:HD2	3:C:2129:HOH:O	1.93	0.52
1:D:742:TRP:O	1:D:745:ILE:HG13	2.10	0.52
1:C:438:CYS:HB2	1:C:439:PRO:CD	2.39	0.51
1:C:516:THR:HB	1:C:517:PRO:HD2	1.93	0.51
1:D:260:ARG:HD3	1:D:590:LEU:HD21	1.92	0.51
1:B:461:GLU:HA	1:B:462:PRO:C	2.35	0.51
1:B:631:LYS:HE2	3:B:3446:HOH:O	2.10	0.51
1:C:512:TRP:CZ3	1:C:554:LEU:HD13	2.45	0.51
1:B:507:HIS:N	1:B:508:PRO:CD	2.73	0.51
1:B:535:VAL:O	1:B:537:PRO:HD3	2.11	0.51
1:C:341:ILE:HG22	1:C:342:PRO:O	2.11	0.51
1:A:392:HIS:CE1	1:A:415:TYR:HB2	2.45	0.51
1:C:364:LEU:HD11	1:C:580:ASN:HB2	1.93	0.51
1:A:31:PRO:HB2	1:A:33:ASP:OD1	2.10	0.51
1:A:604:ALA:HB2	1:A:662:VAL:HG11	1.92	0.51
1:C:592:ALA:O	1:C:594:PRO:HD3	2.10	0.51
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.94	0.51
1:A:461:GLU:HA	1:A:462:PRO:C	2.34	0.51
1:D:507:HIS:N	1:D:508:PRO:HD2	2.25	0.51
1:C:538:TYR:O	1:C:542:ARG:HG3	2.11	0.51
1:D:634:TYR:O	1:D:653:THR:HA	2.11	0.51
1:D:61:ARG:NH1	1:D:66:ASN:HA	2.26	0.51
1:B:392:HIS:ND1	1:B:393:PRO:HD2	2.25	0.50
1:A:411:ARG:HG2	2:A:760:HEM:C2C	2.45	0.50
1:B:521:ARG:HH21	1:B:745:ILE:HG21	1.75	0.50
1:C:552:LEU:HD22	1:C:552:LEU:O	2.10	0.50
1:D:359:LEU:H	1:D:507:HIS:HD2	1.58	0.50
1:B:459:ASN:HD22	1:B:460:TYR:HD2	1.59	0.50
1:C:214:PHE:HB3	1:C:215:PRO:HD3	1.93	0.50
1:C:296:LEU:HD12	1:C:333:GLU:HB3	1.94	0.50
1:A:28:SER:CB	1:D:245:LEU:HD22	2.42	0.50
1:A:562:LEU:HA	1:D:637:MET:HB2	1.94	0.50
1:C:636:ARG:NH2	1:C:639:GLU:O	2.45	0.50
1:D:605:ILE:HD12	1:D:630:ALA:HB1	1.93	0.50
1:B:157:ASN:HB2	3:B:4138:HOH:O	2.12	0.50
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.20	0.50
1:B:116:HIS:CD2	1:D:426:PRO:HB2	2.47	0.49
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ASN:HB2	3:B:2326:HOH:O	2.12	0.49
1:B:207:PHE:CD2	1:B:252:ASN:HB3	2.47	0.49
1:B:378:ASN:HB3	1:B:379:PRO:HD2	1.94	0.49
1:C:542:ARG:NH2	3:C:1922:HOH:O	2.45	0.49
1:A:516:THR:HB	1:A:517:PRO:HD2	1.93	0.49
1:C:296:LEU:HD12	1:C:333:GLU:CB	2.43	0.49
1:A:488:ARG:NE	1:A:490:GLU:OE2	2.34	0.49
1:A:745:ILE:N	1:A:746:PRO:HD2	2.28	0.49
1:D:97:ALA:O	1:D:101:GLY:HA3	2.13	0.49
1:D:751:ILE:HD13	1:D:752:PRO:HD2	1.94	0.49
1:C:505:TYR:HA	1:C:508:PRO:HG2	1.93	0.49
1:C:727:SER:HA	3:C:3714:HOH:O	2.12	0.49
1:C:516:THR:O	1:C:520:GLN:HG3	2.13	0.48
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.94	0.48
1:D:748:ILE:O	1:D:749:ASP:C	2.56	0.48
1:C:222:LYS:HB3	1:C:223:PRO:CD	2.43	0.48
1:A:65:LEU:HD21	1:A:135:HIS:CG	2.49	0.48
1:A:188:LYS:HB2	1:A:391:PHE:CE1	2.48	0.48
1:A:438:CYS:HB2	1:A:439:PRO:HD2	1.93	0.48
1:B:36:HIS:NE2	1:B:37:ARG:HD3	2.29	0.48
1:C:351:PHE:HB2	1:C:358:LYS:HG3	1.95	0.48
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.95	0.48
1:C:125:ARG:HB2	1:C:129:ALA:HA	1.96	0.48
1:C:507:HIS:N	1:C:508:PRO:CD	2.76	0.48
1:A:265:SER:OG	1:A:267:ARG:HB2	2.13	0.48
1:B:174:GLY:O	1:C:231:GLN:HG2	2.13	0.48
1:D:122:ILE:HB	1:D:123:PRO:CD	2.44	0.48
1:A:709:LYS:HE3	1:A:709:LYS:HA	1.96	0.48
1:B:128:HIS:HA	1:B:168:THR:O	2.14	0.48
1:B:745:ILE:HB	1:B:746:PRO:HD3	1.95	0.48
1:C:323:TRP:CZ3	1:C:379:PRO:HD2	2.48	0.48
1:C:335:GLU:OE2	1:C:369:ARG:NH2	2.47	0.48
1:C:621:LYS:NZ	3:C:4070:HOH:O	2.45	0.48
1:B:392:HIS:CE1	1:B:415:TYR:HB2	2.48	0.48
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.49	0.48
1:B:333:GLU:HG2	1:B:374:VAL:HG22	1.96	0.47
1:D:607:LEU:HD22	1:D:611:VAL:HG21	1.96	0.47
1:A:71:VAL:CG2	1:C:453:ILE:HD12	2.44	0.47
1:B:612:ARG:O	1:B:614:ALA:N	2.47	0.47
1:C:392:HIS:CE1	1:C:415:TYR:HB2	2.49	0.47
1:D:750:LYS:HZ2	1:D:750:LYS:HB2	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:ILE:O	1:B:751:ILE:HG22	2.14	0.47
1:B:145:SER:HA	1:B:148:THR:O	2.15	0.47
1:C:516:THR:HB	1:C:517:PRO:CD	2.44	0.47
1:C:643:ASP:OD1	1:C:644:ASP:N	2.47	0.47
1:D:95:LEU:HB3	1:D:107:ASP:HB2	1.96	0.47
1:A:237:ASP:OD2	1:A:536:ARG:HG3	2.13	0.47
1:B:359:LEU:H	1:B:507:HIS:HD2	1.62	0.47
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.49	0.47
1:D:227:TRP:CE3	1:D:229:ILE:HD12	2.48	0.47
1:A:30:ALA:HB1	1:A:31:PRO:HD2	1.97	0.47
1:C:128:HIS:HA	1:C:168:THR:O	2.14	0.47
1:D:309:LYS:HB3	1:D:660:LEU:HD11	1.97	0.47
1:D:323:TRP:CH2	1:D:378:ASN:HB3	2.50	0.47
1:D:583:LYS:HB2	1:D:583:LYS:NZ	2.30	0.47
1:C:610:GLU:HG3	1:C:610:GLU:O	2.15	0.46
1:C:728:PHE:O	1:C:731:GLU:HB2	2.15	0.46
1:B:267:ARG:HG3	3:B:2921:HOH:O	2.15	0.46
1:C:229:ILE:HG23	1:C:230:PRO:HA	1.98	0.46
1:D:392:HIS:ND1	1:D:393:PRO:HD2	2.31	0.46
1:A:83:ASN:HB3	1:C:429:HIS:CD2	2.50	0.46
1:A:693:LYS:HA	1:A:694:PRO:HD3	1.81	0.46
1:B:717:GLY:HA3	1:B:741:VAL:HG11	1.97	0.46
1:D:37:ARG:HA	1:D:38:PRO:HD2	1.76	0.46
1:D:710:ILE:HG23	1:D:715:GLU:HG2	1.98	0.46
1:C:612:ARG:HA	1:C:643:ASP:OD2	2.15	0.46
1:D:418:THR:HG23	1:D:419:GLN:HG3	1.98	0.46
1:D:683:TYR:CD2	1:D:686:MET:HE2	2.51	0.46
1:A:414:SER:HB2	1:D:114:ILE:HG21	1.98	0.46
1:A:689:TYR:OH	1:A:715:GLU:OE2	2.30	0.46
1:B:113:LYS:HD2	3:B:1609:HOH:O	2.16	0.46
1:A:516:THR:O	1:A:520:GLN:HG3	2.16	0.46
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.50	0.46
1:B:563:GLY:HA2	3:B:1767:HOH:O	2.15	0.46
1:B:252:ASN:HD22	1:B:252:ASN:HA	1.55	0.46
1:B:631:LYS:HG3	1:B:633:LEU:HD13	1.97	0.46
1:C:97:ALA:O	1:C:101:GLY:HA3	2.15	0.46
1:C:751:ILE:HG13	1:C:752:PRO:HD2	1.98	0.46
1:A:516:THR:HB	1:A:517:PRO:CD	2.46	0.46
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.50	0.46
1:B:616:LEU:HD23	1:B:616:LEU:HA	1.87	0.46
1:C:43:THR:O	1:C:328:ALA:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.58	0.46
1:C:672:ILE:HD12	1:C:701:ALA:HA	1.97	0.46
1:D:155:ASP:HA	1:D:156:PRO:HD2	1.81	0.46
1:D:607:LEU:O	1:D:675:ILE:HD13	2.16	0.46
1:A:363:GLU:HG2	3:A:2160:HOH:O	2.16	0.45
1:C:278:ARG:HH12	1:C:487:GLU:CD	2.23	0.45
1:A:596:GLY:HA3	1:A:737:ALA:O	2.16	0.45
1:B:253:VAL:O	1:B:254:MET:C	2.60	0.45
1:B:709:LYS:HA	1:B:709:LYS:HD2	1.67	0.45
3:B:1439:HOH:O	1:C:231:GLN:HB2	2.16	0.45
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.99	0.45
1:C:602:VAL:HG12	1:C:603:VAL:N	2.31	0.45
1:D:556:GLN:NE2	3:D:3773:HOH:O	2.50	0.45
1:B:470:PRO:HB2	1:D:80:LEU:HA	1.96	0.45
1:B:593:ILE:HA	1:B:594:PRO:HD2	1.65	0.45
1:C:750:LYS:N	1:C:750:LYS:HE2	2.32	0.45
1:B:331:PHE:HA	1:B:332:PRO:HD3	1.83	0.45
1:C:525:ASP:HB3	3:C:3259:HOH:O	2.16	0.45
1:C:554:LEU:O	1:C:558:VAL:HG23	2.17	0.45
1:A:316:ASP:HB3	1:D:229:ILE:HG12	1.99	0.45
1:D:252:ASN:HD22	1:D:252:ASN:HA	1.53	0.45
1:B:44:PRO:HB3	1:B:629:HIS:CD2	2.52	0.45
1:B:259:ASP:OD1	1:B:522:HIS:ND1	2.47	0.45
1:A:207:PHE:O	1:A:249:THR:HA	2.17	0.45
1:A:262:ILE:HG13	1:A:262:ILE:O	2.17	0.45
1:A:552:LEU:O	1:A:556:GLN:HG3	2.17	0.45
1:A:241:ASP:HB2	1:A:539:ILE:HD13	1.98	0.45
1:A:612:ARG:HA	1:A:643:ASP:OD2	2.16	0.45
1:A:725:ASP:H	1:A:728:PHE:HB3	1.82	0.44
1:A:751:ILE:HD12	1:A:751:ILE:O	2.16	0.44
1:B:170[B]:GLN:HG3	1:B:232:GLY:HA2	1.99	0.44
1:D:87:ARG:HB3	3:D:2379:HOH:O	2.17	0.44
1:A:692:LEU:HD21	1:A:748:ILE:HD13	2.00	0.44
1:D:750:LYS:HD3	1:D:751:ILE:N	2.31	0.44
1:A:637:MET:CG	1:D:532:SER:HB2	2.45	0.44
3:A:1392:HOH:O	1:D:100:ARG:HG3	2.16	0.44
1:D:407:LEU:O	1:D:411:ARG:HG3	2.18	0.44
1:D:461:GLU:HB2	1:D:462:PRO:HA	1.99	0.44
1:A:708:ILE:O	1:A:710:ILE:N	2.51	0.44
1:A:27:ASP:O	1:A:28:SER:C	2.59	0.44
1:C:552:LEU:HD21	1:C:571:LEU:CD1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:604:ALA:HB2	1:D:662:VAL:HG11	1.99	0.44
1:B:369:ARG:HG2	3:B:2639:HOH:O	2.16	0.44
1:B:692:LEU:O	1:B:741:VAL:HG23	2.18	0.44
1:B:720:GLU:O	1:B:721:ALA:HB2	2.17	0.44
1:D:745:ILE:O	1:D:748:ILE:HG12	2.17	0.44
1:A:689:TYR:OH	1:A:710:ILE:HG21	2.18	0.44
1:C:586:PRO:HB2	1:C:593:ILE:HD11	2.00	0.44
1:A:81:THR:O	1:C:442:ASN:HB3	2.18	0.44
1:A:512:TRP:CZ3	1:A:554:LEU:HD13	2.52	0.44
1:A:535:VAL:O	1:A:537:PRO:HD3	2.18	0.44
1:A:282:ALA:HB1	1:A:477:PRO:HB3	1.99	0.44
1:A:331:PHE:O	1:A:333:GLU:HG3	2.18	0.44
1:A:752:PRO:O	1:D:686:MET:HE1	2.18	0.44
1:B:438:CYS:HB2	1:B:439:PRO:HD2	1.98	0.44
1:D:469:TRP:CE3	1:D:471:ARG:HG3	2.53	0.44
1:A:751:ILE:HD13	1:A:753:ALA:HB3	2.00	0.43
1:D:524:VAL:HG22	1:D:554:LEU:HD23	2.00	0.43
1:B:462:PRO:HA	1:B:468:ASN:OD1	2.19	0.43
1:D:750:LYS:HD3	1:D:751:ILE:H	1.82	0.43
1:B:686:MET:SD	1:B:707:THR:HG22	2.58	0.43
1:D:473:THR:O	1:D:481:GLY:HA3	2.18	0.43
1:B:97:ALA:O	1:B:101:GLY:HA3	2.18	0.43
1:C:461:GLU:HA	1:C:462:PRO:C	2.43	0.43
1:A:205:ILE:HD13	1:A:205:ILE:H	1.83	0.43
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.99	0.43
1:A:126:ILE:HD13	1:D:117:PHE:O	2.19	0.43
1:A:533:LYS:NZ	1:D:656:GLY:O	2.47	0.43
1:B:211:ALA:HB3	1:B:410:GLY:HA3	2.00	0.43
1:B:323:TRP:CH2	1:B:378:ASN:HB3	2.54	0.43
1:C:583:LYS:O	1:C:584:LYS:HB3	2.19	0.43
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.53	0.43
1:B:629:HIS:HD2	3:B:1708:HOH:O	2.01	0.43
1:A:459:ASN:HD22	1:A:459:ASN:C	2.27	0.43
1:B:144:LEU:HD11	1:B:370:VAL:HG13	2.01	0.43
1:B:404:ASN:O	1:B:405:ASP:C	2.62	0.43
1:D:179:VAL:HA	3:D:1743:HOH:O	2.19	0.43
1:D:574:THR:OG1	1:D:575:PRO:HD2	2.19	0.43
1:A:86:VAL:HG13	1:C:398:PRO:HD3	2.01	0.43
1:A:369:ARG:NH2	3:A:1391:HOH:O	2.51	0.43
1:B:27:ASP:HB3	3:B:3571:HOH:O	2.19	0.43
1:B:561:ASN:HB3	3:B:3136:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:ASN:HD22	1:D:459:ASN:N	2.12	0.43
1:D:750:LYS:O	1:D:751:ILE:O	2.37	0.43
1:A:29:LEU:HB3	1:C:467:ASP:OD1	2.19	0.42
1:A:710:ILE:HG13	1:A:711:ALA:N	2.34	0.42
1:B:30:ALA:HB1	1:B:31:PRO:HD2	2.01	0.42
1:B:416:THR:HG23	3:B:3659:HOH:O	2.19	0.42
1:C:512:TRP:CH2	1:C:520:GLN:HB3	2.54	0.42
1:A:478:LYS:HE3	3:A:3779:HOH:O	2.19	0.42
1:A:509:ARG:HD2	1:A:576:PRO:HD2	2.00	0.42
1:B:27:ASP:HB3	1:B:28:SER:H	1.36	0.42
1:B:125:ARG:HB2	1:B:129:ALA:HA	2.01	0.42
1:D:668:PRO:HA	1:D:698:ALA:HB3	2.01	0.42
1:A:104:LEU:HB3	3:C:1175:HOH:O	2.18	0.42
1:A:612:ARG:HH22	1:A:723:SER:HB3	1.84	0.42
1:A:689:TYR:HA	1:A:744:ARG:NH1	2.34	0.42
1:B:617:LEU:HA	3:B:3762:HOH:O	2.18	0.42
1:C:331:PHE:HA	1:C:332:PRO:HD3	1.85	0.42
1:A:698:ALA:O	1:A:699:GLY:C	2.63	0.42
1:C:511:PHE:O	1:C:515:GLN:HG2	2.19	0.42
1:D:128:HIS:HA	1:D:168:THR:O	2.18	0.42
1:B:536:ARG:HB3	1:B:538:TYR:CE2	2.54	0.42
1:B:556:GLN:HG2	1:B:566:LEU:CD2	2.48	0.42
1:D:214:PHE:HB3	1:D:215:PRO:HD3	2.00	0.42
1:D:693:LYS:HA	1:D:694:PRO:HD3	1.84	0.42
1:A:145:SER:HA	1:A:148:THR:O	2.19	0.42
1:A:511:PHE:O	1:A:515:GLN:HG2	2.19	0.42
1:B:558:VAL:O	1:B:562:LEU:HD22	2.18	0.42
1:C:314:ASP:HA	1:C:315:PRO:HD2	1.88	0.42
1:C:459:ASN:C	1:C:459:ASN:HD22	2.26	0.42
1:C:488:ARG:HE	1:C:488:ARG:HB2	1.46	0.42
1:D:275:HIS:HB2	1:D:277:PHE:CE2	2.54	0.42
1:B:469:TRP:HA	1:B:470:PRO:C	2.45	0.42
1:B:473:THR:O	1:D:89:ALA:HA	2.20	0.42
1:D:431:ILE:O	1:D:432:PRO:C	2.63	0.42
1:A:335:GLU:OE1	1:A:369:ARG:HD3	2.19	0.42
1:B:48:GLN:HB3	1:B:49:PRO:HD2	2.01	0.42
1:B:345:ASP:OD1	1:B:348:LYS:NZ	2.42	0.42
1:B:354:LEU:O	1:B:356:PRO:HD3	2.20	0.42
1:B:359:LEU:HD12	1:B:359:LEU:C	2.45	0.42
1:B:605:ILE:HG21	1:B:616:LEU:HD21	2.01	0.42
1:B:631:LYS:HG3	1:B:633:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:584:LYS:HB2	1:C:584:LYS:NZ	2.34	0.42
1:D:222:LYS:HB3	1:D:223:PRO:CD	2.50	0.42
1:A:76:GLU:O	1:A:77:ASN:HB2	2.19	0.41
1:A:648:LEU:HA	1:A:649:PRO:HD2	1.91	0.41
1:B:469:TRP:CH2	1:B:471:ARG:HD2	2.55	0.41
1:C:359:LEU:H	1:C:507:HIS:HD2	1.67	0.41
1:A:637:MET:HB2	1:D:562:LEU:HA	2.02	0.41
1:B:309:LYS:HD3	1:C:309:LYS:HE3	2.01	0.41
1:B:672:ILE:HG22	1:B:676:ALA:HB2	2.02	0.41
1:D:702:ARG:O	1:D:705:LYS:HG3	2.20	0.41
1:A:497:ARG:HG2	3:A:1076:HOH:O	2.21	0.41
1:B:678:ASN:OD1	1:B:680:ASP:HB2	2.20	0.41
1:C:490:GLU:HA	1:D:489:VAL:O	2.21	0.41
1:A:583:LYS:HB2	3:A:2913:HOH:O	2.20	0.41
1:B:222:LYS:CB	1:B:223:PRO:CD	2.91	0.41
1:D:574:THR:HG22	3:D:2614:HOH:O	2.20	0.41
1:B:293:TRP:CZ3	1:B:336:LEU:HB2	2.56	0.41
1:D:411:ARG:HG2	2:D:760:HEM:C2C	2.55	0.41
1:D:459:ASN:H	1:D:459:ASN:ND2	2.17	0.41
1:B:413:PHE:HB2	1:D:105:LEU:HD11	2.02	0.41
1:C:686:MET:CB	1:C:751:ILE:HD11	2.50	0.41
1:D:461:GLU:HA	1:D:462:PRO:C	2.45	0.41
1:A:745:ILE:O	1:A:748:ILE:HG12	2.21	0.41
1:B:50:THR:HG21	1:C:227:TRP:CZ3	2.56	0.41
1:B:386:ASN:OD1	1:B:386:ASN:C	2.63	0.41
1:D:132:SER:OG	1:D:319:ARG:HG3	2.20	0.41
1:D:392:HIS:HA	1:D:393:PRO:HD2	1.90	0.41
1:A:330:ASP:OD1	1:A:600:GLY:HA2	2.21	0.41
1:C:660:LEU:HD13	1:C:687:GLU:CD	2.46	0.41
1:D:443:PHE:CE2	1:D:470:PRO:HD2	2.56	0.41
1:B:51:ALA:HB1	1:B:52:PRO:HD2	2.02	0.41
1:B:602:VAL:HG12	1:B:603:VAL:N	2.36	0.41
1:B:615:ASP:O	1:B:616:LEU:C	2.62	0.41
1:C:693:LYS:HA	1:C:694:PRO:HD3	1.94	0.41
1:D:48:GLN:HE21	1:D:48:GLN:HB3	1.64	0.41
1:D:459:ASN:HD22	1:D:460:TYR:HD2	1.69	0.41
1:A:62:ASN:OD1	1:A:62:ASN:C	2.64	0.41
1:B:323:TRP:CZ3	1:B:379:PRO:HD2	2.56	0.41
1:D:392:HIS:HB3	1:D:395:HIS:CE1	2.56	0.41
1:B:643:ASP:OD1	1:B:644:ASP:N	2.54	0.40
1:D:251:HIS:CE1	1:D:507:HIS:HB3	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ARG:HG2	1:D:332:PRO:HB3	2.02	0.40
1:D:392:HIS:CG	1:D:415:TYR:HB2	2.56	0.40
1:D:739:HIS:CD2	1:D:740:ARG:HG2	2.56	0.40
1:B:64:LYS:HE2	1:B:190:TYR:CZ	2.56	0.40
1:C:227:TRP:CE2	1:C:229:ILE:HB	2.56	0.40
1:A:80:LEU:HD12	1:C:442:ASN:HA	2.02	0.40
1:A:155:ASP:HB3	1:A:158:LYS:HB2	2.03	0.40
1:B:337:GLY:HA2	1:B:368:GLN:O	2.20	0.40
1:C:309:LYS:NZ	1:C:687:GLU:OE2	2.46	0.40
1:C:706:ALA:HB3	3:C:3263:HOH:O	2.20	0.40
1:A:345:ASP:O	1:A:346:GLU:C	2.64	0.40
1:B:429:HIS:CG	1:D:83:ASN:HB3	2.56	0.40
1:B:449:HIS:HB2	1:D:449:HIS:CE1	2.56	0.40
1:D:218:VAL:HA	1:D:221:VAL:HG12	2.03	0.40
1:D:669:CYS:SG	1:D:670:GLY:N	2.93	0.40
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.93	0.40
1:A:274:ILE:HD12	2:A:760:HEM:CBB	2.50	0.40
2:A:760:HEM:HBB2	2:A:760:HEM:CMB	2.51	0.40
1:B:476:GLY:HA3	3:B:1270:HOH:O	2.22	0.40
1:C:392:HIS:ND1	1:C:393:PRO:HD2	2.36	0.40
1:C:392:HIS:HA	1:C:393:PRO:HD2	1.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:OD1	1:B:369:ARG:NH1[2_646]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/753 (96%)	697 (96%)	27 (4%)	2 (0%)	36	50
1	B	726/753 (96%)	691 (95%)	29 (4%)	6 (1%)	16	25
1	C	726/753 (96%)	697 (96%)	28 (4%)	1 (0%)	48	64
1	D	726/753 (96%)	694 (96%)	29 (4%)	3 (0%)	30	43
All	All	2904/3012 (96%)	2779 (96%)	113 (4%)	12 (0%)	30	43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	709	LYS
1	B	28	SER
1	B	613	SER
1	D	28	SER
1	D	750	LYS
1	D	751	ILE
1	A	75	SER
1	B	584	LYS
1	C	75	SER
1	B	75	SER
1	B	725	ASP
1	B	594	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	612/635 (96%)	591 (97%)	21 (3%)	32	54
1	B	612/635 (96%)	577 (94%)	35 (6%)	18	33
1	C	612/635 (96%)	577 (94%)	35 (6%)	18	33
1	D	612/635 (96%)	586 (96%)	26 (4%)	26	45
All	All	2448/2540 (96%)	2331 (95%)	117 (5%)	24	40

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	59	ASP
1	A	73	LYS
1	A	170[A]	GLN
1	A	170[B]	GLN
1	A	191	THR
1	A	205	ILE
1	A	252	ASN
1	A	265	SER
1	A	294	LYS
1	A	341	ILE
1	A	375	LEU
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	709	LYS
1	A	712	ASP
1	A	715	GLU
1	A	750	LYS
1	A	751	ILE
1	B	27	ASP
1	B	28	SER
1	B	63	GLU
1	B	126	ILE
1	B	170[A]	GLN
1	B	170[B]	GLN
1	B	198	LEU
1	B	205	ILE
1	B	252	ASN
1	B	283	GLU
1	B	285	LYS
1	B	309	LYS
1	B	370	VAL
1	B	372	LYS
1	B	375	LEU
1	B	377	ARG
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	560	LYS
1	B	562	LEU
1	B	565	GLU

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Mol	Chain	Res	Type
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	610	GLU
1	B	612	ARG
1	B	633	LEU
1	B	639	GLU
1	B	641	THR
1	B	703	LYS
1	B	709	LYS
1	B	732	LEU
1	B	749	ASP
1	B	751	ILE
1	C	32	GLU
1	C	159	ILE
1	C	170[A]	GLN
1	C	170[B]	GLN
1	C	191	THR
1	C	198	LEU
1	C	205	ILE
1	C	252	ASN
1	C	265	SER
1	C	285	LYS
1	C	375	LEU
1	C	377	ARG
1	C	440	TYR
1	C	459	ASN
1	C	488	ARG
1	C	521	ARG
1	C	531	LEU
1	C	552	LEU
1	C	568	ASP
1	C	571	LEU
1	C	584	LYS
1	C	597	ASP
1	C	610	GLU
1	C	612	ARG
1	C	616	LEU
1	C	633	LEU
1	C	635	SER
1	C	648	LEU
1	C	660	LEU

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Mol	Chain	Res	Type
1	C	685	LEU
1	C	713	GLN
1	C	732	LEU
1	C	733	LEU
1	C	747	LYS
1	C	750	LYS
1	D	41	GLU
1	D	73	LYS
1	D	170[A]	GLN
1	D	170[B]	GLN
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	265	SER
1	D	340	LEU
1	D	344	GLU
1	D	375	LEU
1	D	440	TYR
1	D	459	ASN
1	D	552	LEU
1	D	554	LEU
1	D	582	LEU
1	D	598	VAL
1	D	602	VAL
1	D	610	GLU
1	D	633	LEU
1	D	648	LEU
1	D	692	LEU
1	D	747	LYS
1	D	749	ASP
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	459	ASN
1	A	486	GLN
1	A	515	GLN
1	A	520	GLN

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Mol	Chain	Res	Type
1	A	713	GLN
1	B	84	GLN
1	B	157	ASN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	92	GLN
1	C	252	ASN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	572	ASN
1	C	629	HIS
1	D	48	GLN
1	D	252	ASN
1	D	368	GLN
1	D	459	ASN
1	D	507	HIS
1	D	561	ASN
1	D	572	ASN
1	D	629	HIS
1	D	671	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	C	760	1	50,50,50	1.27	5 (10%)	67,82,82	1.09	5 (7%)
2	HEM	A	760	1	50,50,50	1.34	6 (12%)	67,82,82	0.91	2 (2%)
2	HEM	D	760	1	50,50,50	1.23	5 (10%)	67,82,82	0.99	4 (5%)
2	HEM	B	760	1	50,50,50	1.21	4 (8%)	67,82,82	1.14	5 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	760	1	-	4/14/54/54	-
2	HEM	A	760	1	-	2/14/54/54	-
2	HEM	D	760	1	-	2/14/54/54	-
2	HEM	B	760	1	-	2/14/54/54	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	CAC-C3C	2.89	1.55	1.47
2	C	760	HEM	CAC-C3C	2.69	1.54	1.47
2	D	760	HEM	FE-ND	2.68	2.03	1.94
2	A	760	HEM	CMB-C2B	2.52	1.55	1.50
2	B	760	HEM	CAB-C3B	2.50	1.54	1.47
2	D	760	HEM	CAB-C3B	2.46	1.54	1.47
2	C	760	HEM	CAB-C3B	2.46	1.54	1.47
2	D	760	HEM	C2A-C3A	-2.45	1.32	1.38
2	C	760	HEM	FE-ND	2.32	2.02	1.94
2	A	760	HEM	CAB-C3B	2.31	1.53	1.47
2	A	760	HEM	FE-NA	2.26	2.02	1.95
2	C	760	HEM	FE-NB	2.21	2.01	1.94
2	A	760	HEM	FE-NC	2.20	2.02	1.95
2	B	760	HEM	CAC-C3C	2.20	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760	HEM	CAC-C3C	2.20	1.53	1.47
2	B	760	HEM	FE-NA	2.15	2.02	1.95
2	B	760	HEM	C2A-C3A	-2.13	1.33	1.38
2	D	760	HEM	FE-NA	2.11	2.02	1.95
2	A	760	HEM	FE-NB	2.10	2.01	1.94
2	C	760	HEM	C3D-C2D	-2.09	1.32	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	760	HEM	O1A-CGA-CBA	-2.93	113.81	123.09
2	D	760	HEM	O2A-CGA-O1A	2.81	130.56	123.33
2	A	760	HEM	CHD-C4C-NC	2.68	127.38	124.45
2	B	760	HEM	CMD-C2D-C1D	-2.54	121.07	125.03
2	B	760	HEM	CBA-CAA-C2A	2.41	119.20	112.53
2	A	760	HEM	O1A-CGA-CBA	-2.38	115.54	123.09
2	C	760	HEM	CMA-C3A-C2A	2.29	130.49	125.62
2	C	760	HEM	CHC-C1C-NC	2.29	126.95	124.45
2	D	760	HEM	CHC-C4B-NB	2.23	126.83	124.42
2	B	760	HEM	CMD-C2D-C3D	2.18	132.05	126.15
2	D	760	HEM	CBA-CAA-C2A	2.16	118.51	112.53
2	C	760	HEM	O1D-CGD-CBD	-2.15	116.28	123.09
2	C	760	HEM	O1A-CGA-CBA	-2.12	116.38	123.09
2	C	760	HEM	CMA-C3A-C4A	-2.10	122.22	125.42
2	B	760	HEM	CBB-CAB-C3B	-2.09	117.06	127.53
2	B	760	HEM	CHB-C4A-NA	2.06	127.59	123.86

There are no chirality outliers.

All (10) torsion outliers are listed below:

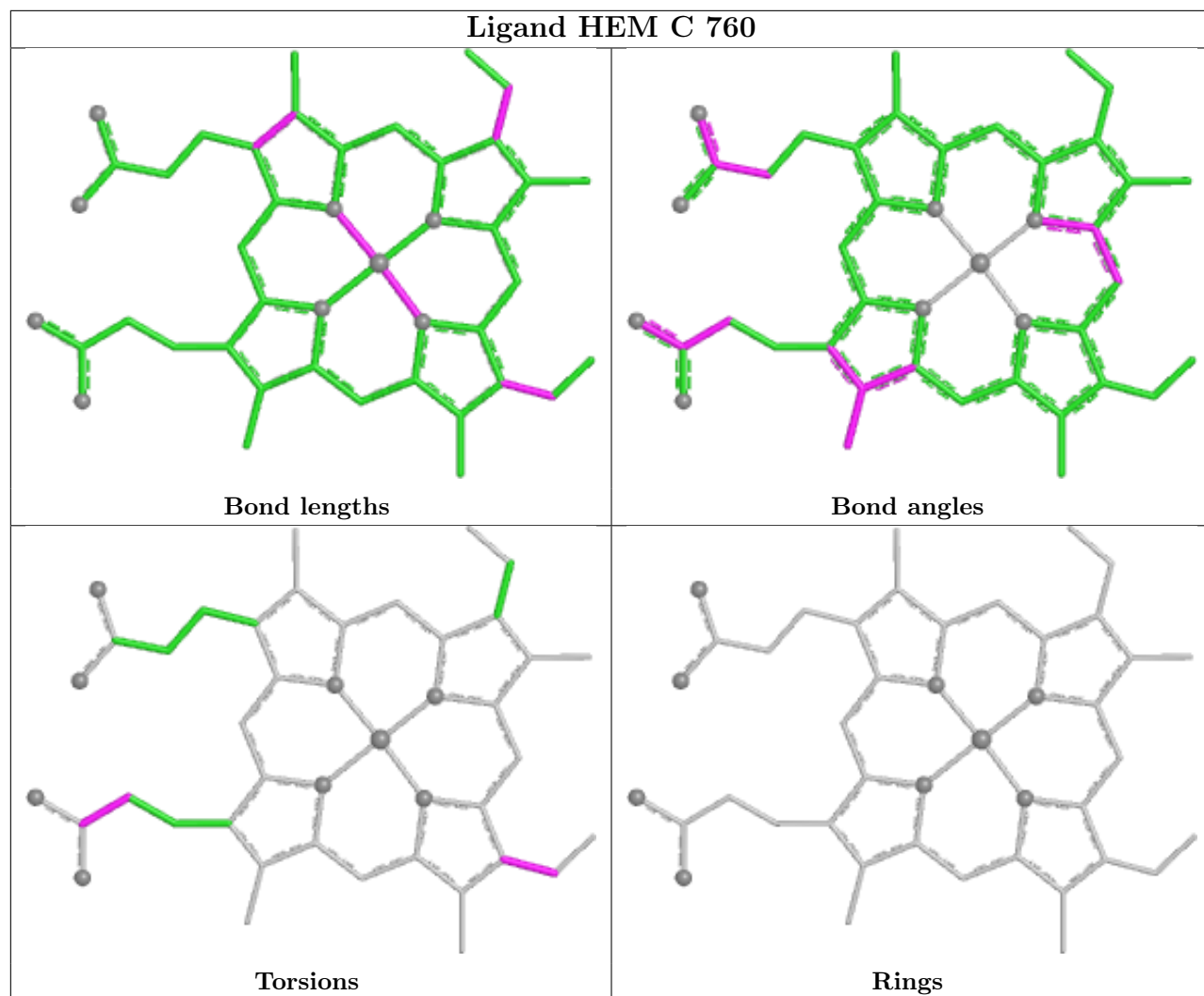
Mol	Chain	Res	Type	Atoms
2	C	760	HEM	C2B-C3B-CAB-CBB
2	C	760	HEM	C4B-C3B-CAB-CBB
2	B	760	HEM	CAA-CBA-CGA-O2A
2	C	760	HEM	CAA-CBA-CGA-O2A
2	B	760	HEM	CAA-CBA-CGA-O1A
2	D	760	HEM	CAA-CBA-CGA-O2A
2	C	760	HEM	CAA-CBA-CGA-O1A
2	A	760	HEM	CAA-CBA-CGA-O1A
2	A	760	HEM	CAA-CBA-CGA-O2A
2	D	760	HEM	CAA-CBA-CGA-O1A

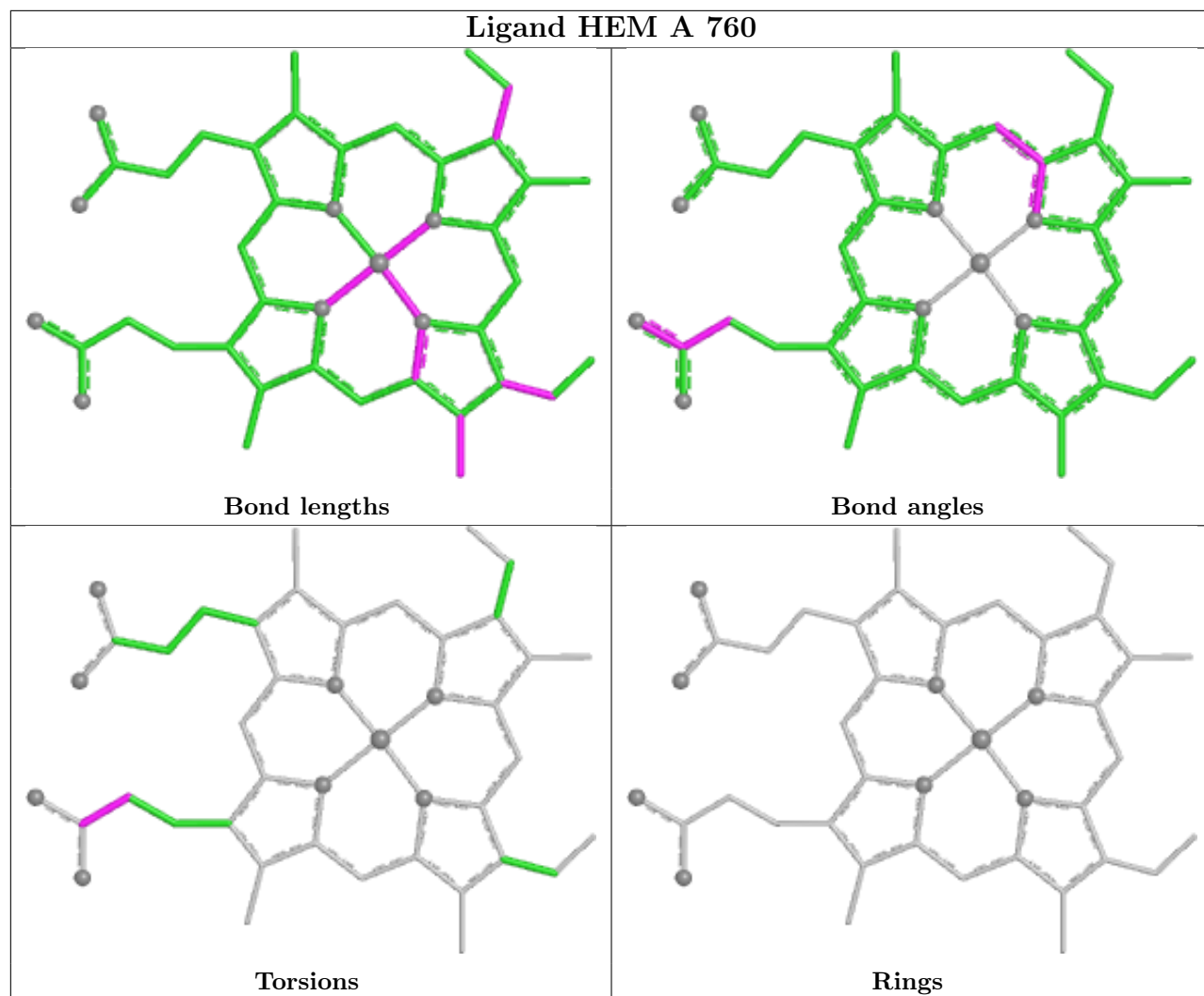
There are no ring outliers.

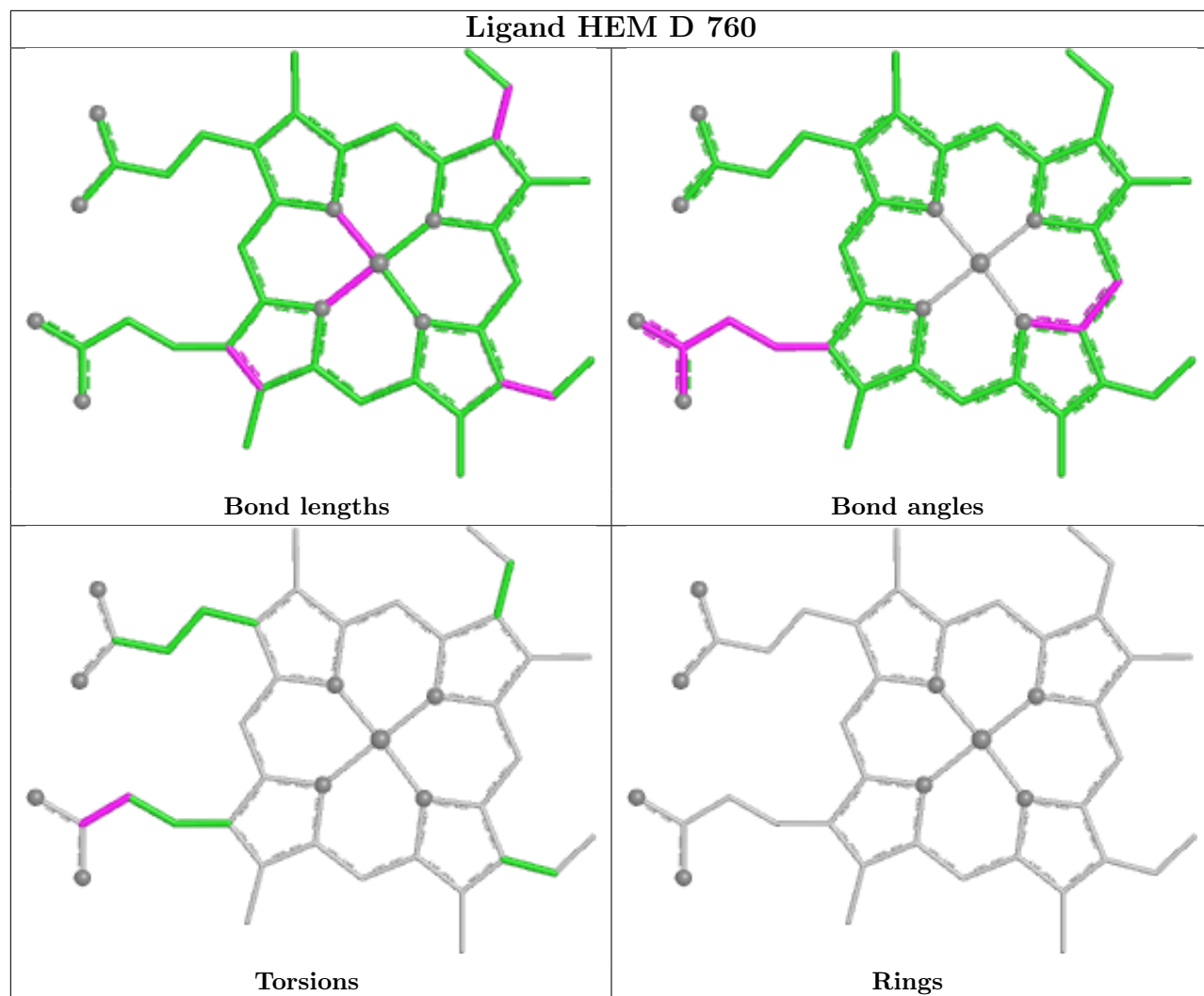
4 monomers are involved in 12 short contacts:

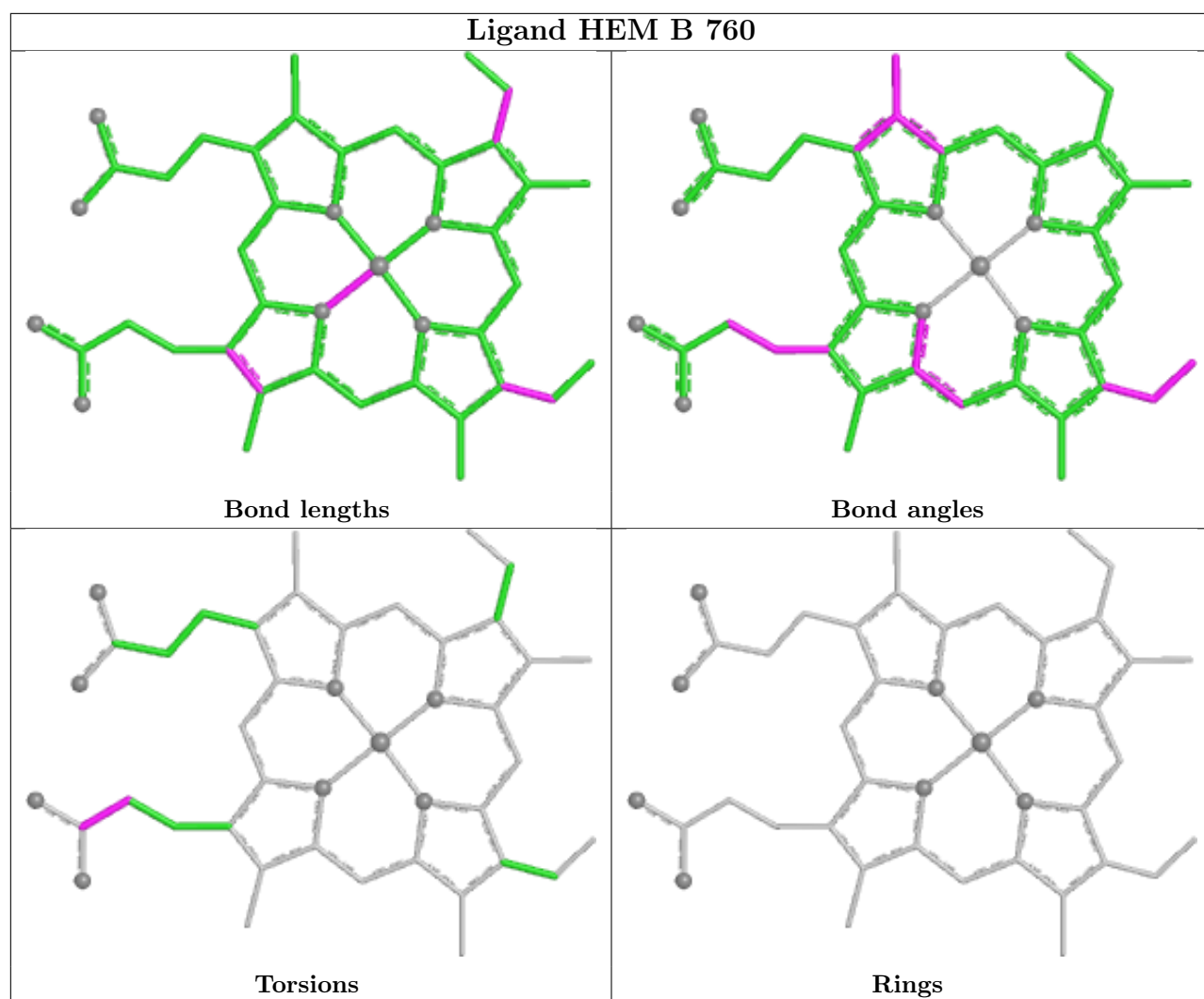
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	760	HEM	3	0
2	A	760	HEM	6	0
2	D	760	HEM	2	0
2	B	760	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	727/753 (96%)	0.77	38 (5%)	33 29	13, 23, 43, 70	2 (0%)
1	B	727/753 (96%)	0.23	6 (0%)	82 80	14, 24, 48, 66	2 (0%)
1	C	727/753 (96%)	0.31	8 (1%)	78 74	15, 24, 47, 64	2 (0%)
1	D	727/753 (96%)	0.93	47 (6%)	25 21	15, 23, 44, 64	2 (0%)
All	All	2908/3012 (96%)	0.56	99 (3%)	48 44	13, 23, 46, 70	8 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	SER	6.1
1	C	27	ASP	4.9
1	A	710	ILE	4.5
1	A	27	ASP	4.1
1	B	27	ASP	4.1
1	C	284	GLY	3.6
1	D	724	ALA	3.5
1	D	27	ASP	3.5
1	A	738	ALA	3.4
1	D	748	ILE	3.2
1	C	28	SER	3.2
1	A	708	ILE	3.1
1	A	712	ASP	3.1
1	D	714	GLY	3.1
1	A	749	ASP	3.0
1	D	719	VAL	3.0
1	D	511	PHE	3.0
1	D	711	ALA	2.9
1	A	30	ALA	2.9
1	D	514	SER	2.9
1	D	723	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	672	ILE	2.8
1	D	371	GLY	2.8
1	A	711	ALA	2.8
1	A	689	TYR	2.7
1	A	329	GLY	2.7
1	A	704	PHE	2.7
1	D	134	ALA	2.7
1	D	721	ALA	2.7
1	A	29	LEU	2.6
1	D	671	ASN	2.6
1	A	709	LYS	2.6
1	D	655	ALA	2.6
1	D	516	THR	2.6
1	A	725	ASP	2.5
1	A	679	GLY	2.5
1	C	476	GLY	2.5
1	A	751	ILE	2.5
1	D	745	ILE	2.5
1	D	752	PRO	2.5
1	D	368	GLN	2.5
1	A	614	ALA	2.5
1	D	326	ILE	2.4
1	D	598	VAL	2.4
1	A	592	ALA	2.4
1	D	559	ALA	2.4
1	D	46	GLY	2.4
1	A	643	ASP	2.4
1	C	481	GLY	2.3
1	D	710	ILE	2.3
1	A	680	ASP	2.3
1	D	549	HIS	2.3
1	A	618	ALA	2.3
1	A	707	THR	2.3
1	A	609	ASP	2.3
1	A	722	ASP	2.3
1	A	76	GLU	2.3
1	D	552	LEU	2.3
1	D	568	ASP	2.3
1	D	38	PRO	2.3
1	B	30	ALA	2.2
1	D	623	LEU	2.2
1	A	612	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	449	HIS	2.2
1	C	751	ILE	2.2
1	A	668	PRO	2.2
1	A	53	GLY	2.2
1	A	649	PRO	2.2
1	A	676	ALA	2.2
1	D	627	GLY	2.2
1	D	708	ILE	2.2
1	A	31	PRO	2.2
1	D	696	ALA	2.1
1	D	609	ASP	2.1
1	D	749	ASP	2.1
1	B	752	PRO	2.1
1	D	253	VAL	2.1
1	D	650	ILE	2.1
1	B	568	ASP	2.1
1	D	686	MET	2.1
1	D	582	LEU	2.1
1	A	600	GLY	2.1
1	B	37	ARG	2.1
1	A	716	GLU	2.1
1	D	523	ILE	2.1
1	A	691	HIS	2.1
1	A	622	ALA	2.0
1	D	555	ALA	2.0
1	D	606	LEU	2.0
1	D	608	ASN	2.0
1	D	563	GLY	2.0
1	D	43	THR	2.0
1	C	594	PRO	2.0
1	D	145	SER	2.0
1	A	744	ARG	2.0
1	D	614	ALA	2.0
1	A	653	THR	2.0
1	B	751	ILE	2.0
1	D	301	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

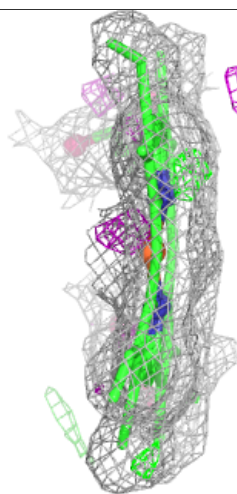
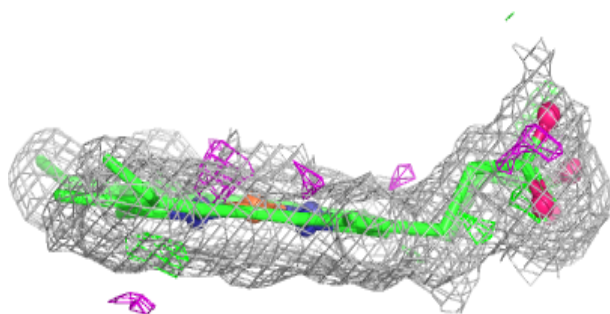
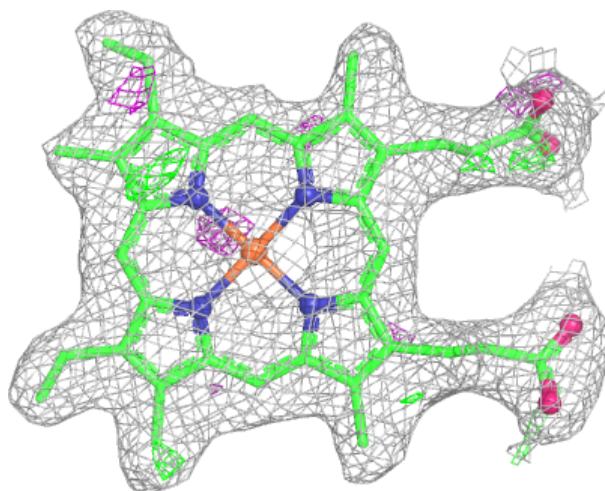
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	A	760	43/43	0.91	0.13	14,18,20,21	0
2	HEM	C	760	43/43	0.92	0.11	18,19,22,23	0
2	HEM	D	760	43/43	0.93	0.10	14,16,19,21	0
2	HEM	B	760	43/43	0.95	0.09	15,17,19,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

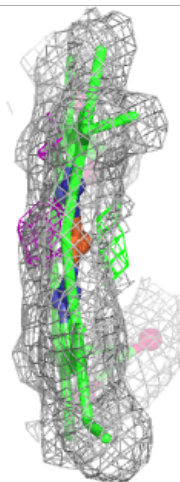
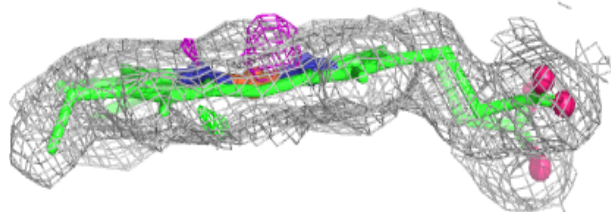
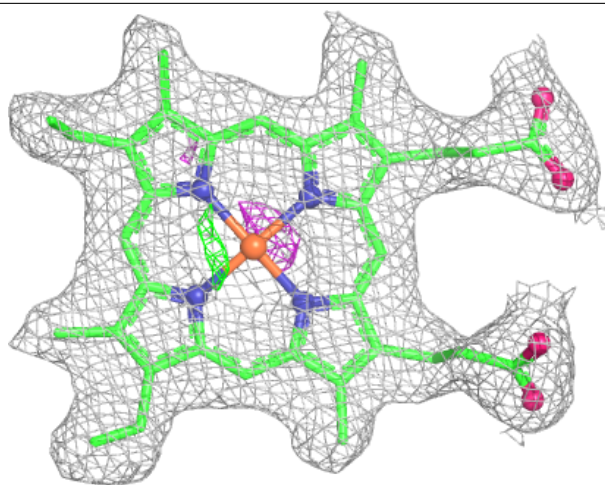
Electron density around HEM A 760:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



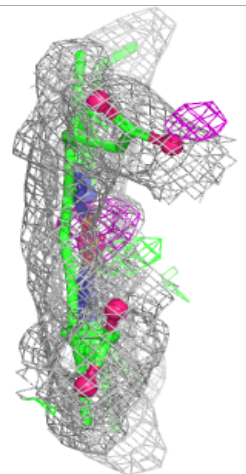
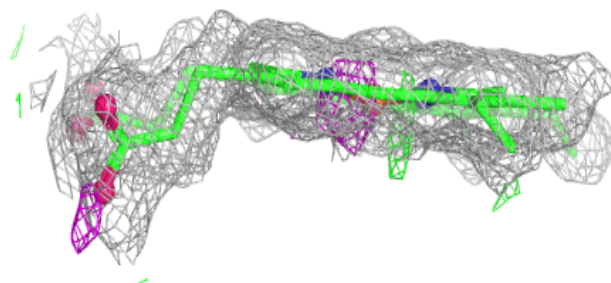
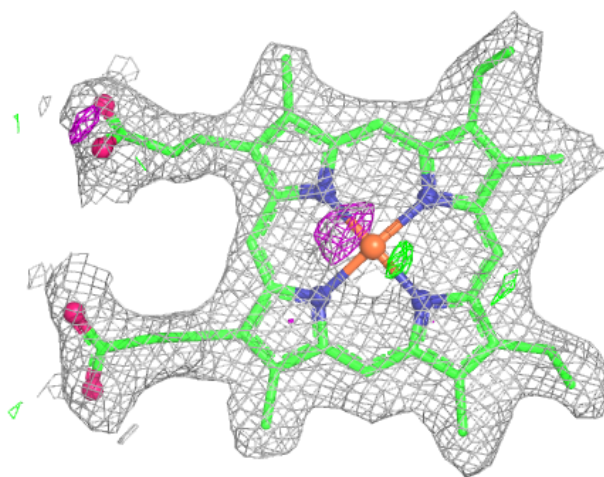
Electron density around HEM C 760:

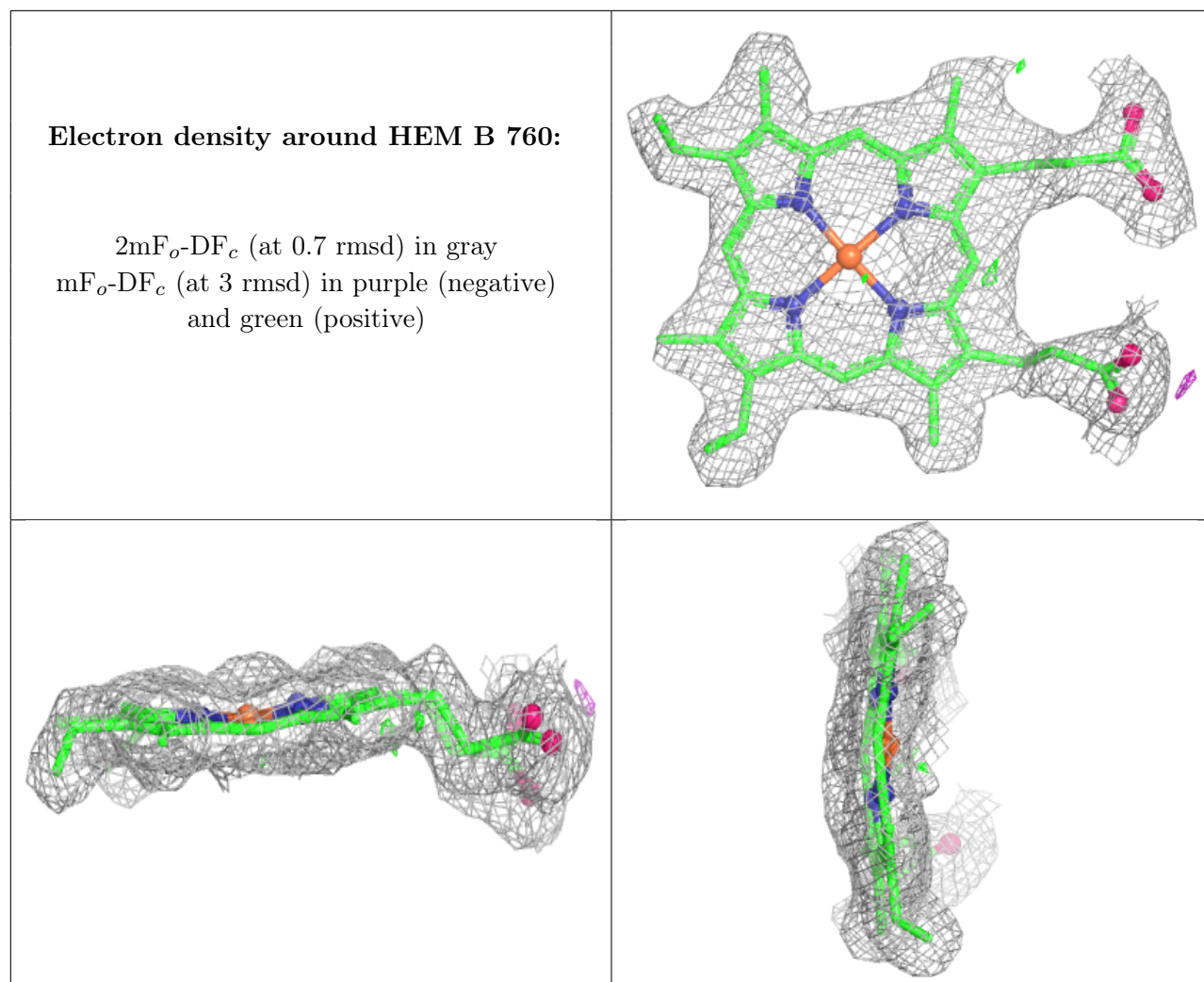
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM D 760:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.